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Solution of the Fokker–Planck Equation for the Shock Wave Problem

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An eigenexpansion solution of the time-independent Brownian motion Fokker–Planck equation is given for a situation in which the external acceleration is a step function. The solution describes the heavy-species velocity distribution function in a binary mixture undergoing a shock wave, in the limit of high dilution of the heavy species and negligible width of the light-gas internal shock. The diffusion solution is part of the eigenexpansion. The coefficients of the series of eigenfunctions are obtained analytically with transcendentally small errors of order $\exp(-1/M)$, where $M \ll 1$ is the mass ratio. Comparison is made with results from a hypersonic approximation.

KEY WORDS: Fokker–Planck equation; shock wave; Brownian motion; eigentheory.

1. INTRODUCTION

The evolution of heavy molecules diluted in a host light gas can be described at the kinetic level by the same Fokker–Planck (FP) equation governing the Brownian motion of particles. Although this equation has its origin in the theory of stochastic processes,[2] it also applies to the heavy molecules in a binary mixture and can be derived from the Boltzmann equation of the heavy gas (which is assumed very dilute, so that heavy–heavy collisions may be neglected) by expanding the cross-collision integral in powers of the molecular mass ratio M ($M = m/m_p \ll 1$, where m is the

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[2] See, for instance, the compilation of review papers edited by Wax[(1)] and the work of Kramers,[(2)] or the derivation given in the textbook of Résibois and De Leener.[(3)] Extensions of the FP equation to a nonequilibrium host gas, from the stochastic point of view, were made by Mazo[(4)] and Slinn and Shen.[(5)]

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molecular weight and the subscript p stands for the heavy species or particles). This expansion was carried out by Wang Chang and Uhlenbeck[6] for the case when the light gas is in equilibrium, and extended to a non-equilibrium host gas by Fernandez de la Mora *et al.*[7,8]

When the difference between the species mean velocity is small compared with the light-gas sound speed, the FP equation for the heavy-species velocity distribution function $f(\mathbf{u}, \mathbf{x}, t)$ reads[7]

$$\partial_t f + \mathbf{u} \cdot \nabla f = \tau^{-1} \nabla_u \cdot [(\mathbf{u} - \mathbf{W}) f + (kT/m_p) \nabla_u f] \tag{1}$$

where k is Boltzmann's constant, $T(\mathbf{x}, t)$ is the light-gas temperature, and $\mathbf{W}(\mathbf{x}, t)$ is given by

$$\mathbf{W} = \mathbf{U} + D\alpha_T \nabla \ln T \tag{2}$$

while $\mathbf{U}(\mathbf{x}, t)$ is the light-gas velocity, α_T is the thermal diffusion ratio,[9] and D is the binary diffusion coefficient, related to the relaxation time τ entering into Eq. (1) by Einstein's law:

$$\tau = m_p D/kT \tag{3}$$

The driving force $\mathbf{W}/\tau$ due to the motion of the light gas plays here the same role as the external acceleration arising in the theory of stochastic processes.[1]

In the particular case in which $\mathbf{W}$ is a constant, the solution of Eq. (1) for stationary problems can be expressed as an eigenexpansion,[10,11] which must be completed by adding a so-called diffusion solution,[12,2,13-18] since, in general, the system of eigenfunctions is not complete.[14] However, in most cases, due to the peculiar form of the boundary conditions, the coefficients of the eigenexpansion have to be calculated by complicated numerical algorithms.[13,15,19-21] For instance, in the case of an absorbing boundary at $x = 0$, $f(x = 0) = 0$ for $u_x > 0$. Since the orthogonality properties of the eigenfunctions are in general extended to all the values of u_x $(-\infty < u_x < +\infty)$, they cannot be used to determine the coefficients in the eigenexpansion.[3] The same difficulty arises for perfectly reflecting and mixed boundaries. The numerical task of obtaining these coefficients by such methods is then enormous, since a very large number of eigenfunctions is needed to reach a reasonably good precision, particularly near

[3] Half-range orthogonality properties with a weight function similar to the Chandrasekhar H function for the neutron transport problem have been proposed to obtain these coefficients.[22] However, no such weight function has been found, to our knowledge, for any problem involving the Fokker–Planck equation.

the boundaries[15] (sufficiently far from the boundaries, the diffusion solution is, in most cases, a good approximation to the exact solution).

In the present paper, we give an analytic "almost exact" solution [with an error of order $\exp(-1/M)$, $M \ll 1$][4] of Eq. (1) in a situation in which $\mathbf{W}$, T, and τ change discontinuously at $x=0$, taking constant values in the intervals $-\infty < x < 0$ and $0 < x < +\infty$. Physically, the problem models a situation in which the light gas undergoes a normal shock of zero thickness and the heavy species is highly diluted ($n_p/n \ll 1$, where n and n_p are the number densities of the light and heavy species, respectively). The eigenexpansion coefficients are obtained analytically via orthogonality properties {within the error $O[\exp(-1/M)]$}, while the diffusion solution is contained in the eigenexpansion.

In addition to its mathematical interest, the present work yields a nearly exact kinetic description of the far-from-equilibrium behavior of disparate-mass mixtures in a regime where they are of considerable industrial importance. Our results thus yield a standard against which other approximate theories may be tested, as we show in Section 3 for the hypersonic method of closure of the hydrodynamic equations.[23–25]

2. SOLUTION OF THE FOKKER–PLANCK EQUATION FOR THE SHOCK WAVE PROBLEM

Consider the one-dimensional steady flow of a disparate-mass binary mixture with supersonic velocity U_0 and temperature T_0. By self-collisions, the light gas is decelerated to a velocity U and its temperature increases to a value T in a distance which, roughly, is m/m_p times shorter than that needed by the heavy gas to equilibrate with the light gas by cross-collisions. Therefore, the light-gas shock wave may be considered, in first approximation in the mass ratio m/m_p, as a discontinuity occurring at $x=0$. Moreover, since n_p/n is very small, the post-shock values of the light-gas velocity and temperature U and T are assumed constants through the relaxation zone $x>0$ (see, e.g., Fig. 1). Thus, the Fokker–Planck equation (1) for the heavy-gas velocity distribution functions $f^-(x<0)$ and $f^+(x>0)$ can be written as

$$\tau_0 u_x \, \partial_x f^- = \nabla_u \cdot [(\mathbf{u} - U_0 \mathbf{e}_x) f^- + (kT_0/m_p) \nabla_u f^-], \qquad x<0 \quad (4)$$

$$\tau u_x \, \partial_x f^+ = \nabla_u \cdot [(\mathbf{u} - U \mathbf{e}_x) f^+ + (kT/m_p) \nabla_u f^+], \qquad x>0 \quad (5)$$

where $\mathbf{e}_x$ is the unit vector in the x direction and the relaxation times τ and

[4] For He–Ar mixtures ($M=0.1$), $\exp(-1/M)=4.54\times 10^{-5}$; for He–Xe ($M=0.031$), $\exp(-1/M)=9.78\times 10^{-15}$.

τ_0 are given by Eq. (3) evaluated at post-shock and pre-shock conditions, respectively. U and U_0, and T and T_0, are connected through the Rankine–Hugoniot conditions

$$U/U_0 = [M_1^2(\gamma - 1) + 2]/(\gamma + 1)\, M_1^2 \tag{6}$$

$$T/T_0 = 1 + 2(\gamma - 1)(M_1^2 - 1)(\gamma M_1^2 + 1)/(\gamma + 1)^2\, M_1^2 \tag{7}$$

where γ $(=5/3)$ is the specific heat ratio of the light gas and M_1 is the Mach number based on the upstream light gas conditions:

$$M_1^2 = U_0^2/(\gamma k T_0/m) \tag{8}$$

The boundary conditions for Eqs. (4) and (5) are

$$f^- = n_{p0}(m_p/2\pi k T_0)^{3/2} \exp[-(m_p/2kT_0)\,|\mathbf{u} - U_0\mathbf{e}_x|^2], \quad \text{as } x \to -\infty \tag{9}$$

$$f^+ = n_{p\infty}(m_p/2\pi k T)^{3/2} \exp[-(m_p/2kT)\,|\mathbf{u} - U\mathbf{e}_x|^2], \quad \text{as } x \to +\infty \tag{10}$$

$$f^-(x=0) = f^+(x=0) \tag{11}$$

that is, as $x \to -\infty$ and $x \to +\infty$, f^- and f^+ are Maxwellian distributions with number densities, mean velocities, and temperatures n_{p0}, U_0, T_0 and $n_{p\infty}$, U, T, respectively. (The number densities are related to the mean velocity through the continuity equation $n_{p0} U_0 = n_{p\infty} U$).

It is convenient to write Eqs. (4) and (5) in polar cylindrical coordinates in velocity space with polar axis directed along $\mathbf{e}_x$. On using the dimensionless variables

$$\xi^+ = u_x/(2kT/m_p)^{1/2} \tag{12}$$

$$\eta^+ = (u_y^2 + u_z^2)^{1/2}/(2kT/m_p)^{1/2} \tag{13}$$

$$y^+ = x/\tau(2kT/m_p)^{1/2} \tag{14}$$

for $x > 0$, and similarly ξ^-, η^-, and y^- with T_0 and τ_0 instead of T and τ for $x < 0$, Eqs. (4) and (5) become

$$\xi^+\, \partial f^+/\partial y^+ = (\xi^+ - V)\, \partial f^+/\partial \xi^+ + \eta^+\, \partial f^+/\partial \eta^+ + 3f^+ + \tfrac{1}{2}[\partial^2 f^+/\partial \xi^{+2} + \partial^2 f^+/\partial \eta^{+2} + (\partial f^+/\partial \eta^+)/\eta^+] \tag{15}$$

where

$$V = U/(2kT/m_p)^{1/2} \tag{16}$$

and similarly for $x<0$ but with ξ^-, η^-, f^-, y^-, and

$$V_0 = U_0/(2kT_0/m_p)^{1/2} \tag{17}$$

instead of ξ^+, η^+, f^+, y^+, and V. [Notice that V_0 is a large number of order $M^{-1/2}$ since $U_0 > (\gamma k T_0/m)^{1/2}$.]

Equation (15) and its counterpart for $x<0$ can be separated. Since both equations are completely similar, we will only consider the equation for $x>0$, dropping the superscript + for the moment. Defining the functions $H(\xi)$ and $L(z)$ (where $z \equiv \eta^2$) as

$$f(\xi, \eta, y) = H(\xi)\, L(z) \exp[-(\xi - V - \gamma/2)^2 - z - \gamma y]$$

with γ an arbitrary constant [not to be confused with the ratio of specific heats in Eqs. (6)–(8)], after substituting into Eq. (15), these functions satisfy the ordinary differential equations

$$H'' - 2(\xi - V - \gamma)\, H' + [\gamma(\gamma + 2V) - 2C]\, H = 0 \tag{18}$$

$$zL'' + (1 - z)\, L' + (C/2)\, L = 0 \tag{19}$$

where C and γ are separation constants. By choosing

$$\begin{aligned} C &= 2m, \qquad m = 0, 1, 2,... \\ \gamma(\gamma + 2V) - 2C &= 2n, \qquad n = 0, 1, 2,... \end{aligned} \tag{20}$$

we have that Eqs. (18) and (19) become Hermite and Laguerre equations of order n and m, respectively.[26] Hence the solution of Eq. (15) for $x>0$ may be written as the expansion

$$\begin{aligned} f^+ = &\sum_{nm} a^+_{nm} H_n(\xi^+ - V - \gamma^+_{nm})\, L_m(\eta^{+2}) \\ &\times \exp[-(\xi^+ - V - \gamma^+_{nm}/2)^2 - \eta^{+2} - \gamma^+_{nm}\, y^+] \\ &+ \sum_{nm} b^+_{nm} H_n(\xi^+ - V - \gamma^-_{nm})\, L_m(\eta^{+2}) \\ &\times \exp[-(\xi^+ - V - \gamma^-_{nm}/2)^2 - \eta^{+2} - \gamma^-_{nm}\, y^+] \end{aligned} \tag{21}$$

where H_n and L_m are the Hermite and Laguerre polynomials of degree n and m; $\gamma^\pm_{nm}$ is given [from Eq. (20)] by

$$\gamma^\pm_{nm} = -V \pm (V^2 + 4m + 2n)^{1/2} \tag{22}$$

and the coefficients a_{nm}^{+} and b_{nm}^{+} are arbitrary constants. Similarly,

$$\begin{aligned} f^{-} = & \sum_{nm} a_{nm}^{-} H_n(\xi^{-} - V_0 - \gamma_{nm}^{0+})\, L_m[(\eta^{-})^2] \\ & \times \exp[-(\xi^{-} - V_0 - \gamma_{nm}^{0+}/2)^2 - (\eta^{-})^2 - \gamma_{nm}^{0+} y^{-}] \\ & + \sum_{nm} b_{nm}^{-} H_n(\xi^{-} - V_0 - \gamma_{nm}^{0-})\, L_m[(\eta^{-})^2] \\ & \times \exp[-(\xi^{-} - V_0 - \gamma_{nm}^{0-}/2)^2 - (\eta^{-})^2 - \gamma_{nm}^{0-} y^{-}] \end{aligned} \tag{23}$$

where

$$\gamma_{nm}^{0\pm} = -V_0 \pm (V_0^2 + 4m + 2n)^{1/2} \tag{24}$$

The two eigenfunctions corresponding to $n = m = 0$ can be identified with the equilibrium Maxwellians and with the so-called diffusion solution to Eqs. (4) and (5). This last function is the product of a Maxwellian and a function of the single variable $x - \tau u_x$, and must be added to the system of eigenfunctions resulting from separating variables in order to make it complete.[12–14] The function $(x - \tau u_x)\exp(-m_p u^2/2kT)$ is the diffusion solution for the one-dimensional problem in a medium at rest.[15] For the present case, the diffusion solution is not linear but exponential in the group $x - \tau u_x$. As a result, exceptionally, it is separable and is already included within the eigenexpansions as

$$f_{\text{diff}}^{+} = a_1 \exp[2V(y^{+} - \xi^{+})] \exp[-(\xi^{+} - V)^2 - (\eta^{+})^2] \tag{25}$$

$$f_{\text{diff}}^{-} = A_1 \exp[2V_0(y^{-} - \xi^{-})] \exp[-(\xi^{-} - V_0)^2 - (\eta^{-})^2] \tag{26}$$

where a_1 and A_1 are constants [notice the correspondence between these functions and the terms in Eqs. (21) and (23) whose constants are b_{00}^{+} and b_{00}^{-}, respectively].

Since the γ_{nm}^{-} are negative constants, the coefficients b_{nm}^{+} must be equal to zero in order for f^{+} to be bound as $y^{+} \to \infty$. A similar condition for f^{-} as $y^{-} \to -\infty$ implies that all $a_{nm}^{-} = 0$, except for a_{00}^{-}. From the boundary conditions (9) and (10),

$$a_{00}^{+} = n_{p\infty}(m_p/2\pi kT)^{3/2} \tag{27}$$

$$a_{00}^{-} = n_{p0}(m_p/2\pi kT_0)^{3/2} \tag{28}$$

The remaining constants a_{nm}^{+}, n, $m \neq 0$, and b_{nm}^{-} may be obtained by making use of the boundary condition (11) and the orthogonality properties of H_n and L_m.

Instead of the orthogonality properties of the functions H_n, it is advantageous to use those of the functions

$$G_{nm}^{\pm}(\xi) \equiv \exp[-(\xi - V - \gamma_{nm}^{\pm}/2)^2] \, H_n(\xi - V - \gamma_{nm}^{\pm}) \tag{29}$$

$$G_{nm}^{0\pm}(\xi) \equiv \exp[-(\xi - V_0 - \gamma_{nm}^{0\pm}/2)^2] \, H_n(\xi - V_0 - \gamma_{nm}^{0\pm}) \tag{30}$$

which are given in the Appendix. A consequence of the orthogonality properties of these functions G is that only the term a_{00}^{+} in Eq. (21) and the term a_{00}^{-} in Eq. (23) (corresponding to $\gamma_{00}^{+} = \gamma_{00}^{0+} = 0$) contribute to the flow. Thus, substituting the expansions (21) and (23) into the condition (11), multiplying by $\eta^{+}\xi^{+} \, d\xi^{+} \, d\eta^{+}$, and integrating over velocity space (between 0 and ∞ for η and between $-\infty$ and $+\infty$ for ξ), one obtains the continuity equation $n_{p0} U_0 = n_{p\infty} U$, where use has been made of Eqs. (27) and (28). On the other hand, multiplying by

$$2\eta^{+} L_m(\eta^{+2}) \exp[(\xi^{+} - V)^2] \, \xi^{+} G_{nm}^{+}(\xi^{+}) \, d\xi^{+} \, d\eta^{+}$$

and integrating over velocity space, one gets

$$A_{nm} a_{nm}^{+} = \sum_{ij} B_{nmij} b_{ij}^{-} + C_{nm} a_{00}^{-} \tag{31}$$

where

$$A_{nm} = \theta^2 \exp[(\gamma_{nm}^{+})^2/2] \, (V + \gamma_{nm}^{+}) \sqrt{\pi} \, 2^n n! \tag{32}$$

$$B_{nmij} = 2 \int_0^{+\infty} dx \, x L_m(x^2/\theta) \, L_j(x^2) \exp(-x^2) \times \int_{-\infty}^{+\infty} dx \, x \exp[(x/\theta^{1/2} - V)^2] \, G_{nm}^{+}(x/\theta^{1/2}) \, G_{ij}^{0-}(x) \tag{33}$$

$$C_{nm} = 2 \int_0^{+\infty} dx \, x L_m(x^2/\theta) \exp(-x^2) \int_{-\infty}^{+\infty} dx \times x \exp[(x/\theta^{1/2} - V)^2] \, G_{nm}^{+}(x/\theta^{1/2}) \exp[-(x - V_0)^2] \tag{34}$$

and

$$\theta = T/T_0 \tag{35}$$

Similarly, multiplying Eq. (11) by

$$2\eta^{-} L_m[(\eta^{-})^2] \exp[(\xi^{-} - V_0)^2] \, \xi^{-} G_{nm}^{0-}(\xi^{-}) \, d\xi^{-} \, d\eta^{-}$$

and integrating over velocity space, we have

$$D_{nm} b_{nm}^{-} = \sum_{kl} E_{nmkl} a_{kl}^{+} \tag{36}$$

where

$$D_{nm} = \theta^{-2} \exp[(\gamma_{nm}^{0-})^2/2] \, (V_0 + \gamma_{nm}^{0-}) \sqrt{\pi}\, 2^n n! \tag{37}$$

$$E_{nmkl} = 2 \int_0^{+\infty} dx\, x L_m(x^2\theta)\, L_l(x^2) \exp(-x^2) \times \int_{-\infty}^{+\infty} dx\, x \exp[(x\theta^{1/2} - V_0)^2]\, G_{nm}^{0-}(x\theta^{1/2})\, G_{kl}^{+}(x) \tag{38}$$

To obtain the above expressions, use has been made of the properties given in the Appendix (notice that $\eta^- = \theta^{1/2}\eta^+$ and $\xi^- = \theta^{1/2}\xi^+$).

The infinite system of algebraic equations (31) or (36) may be solved by successive approximations. For instance, one can make a guess for the coefficients b_{nm}^- and use the equation [combination of (31) and (36)]

$$D_{ij} b_{ij}^- = \left[\sum_{kl} E_{ijkl} \left(a_{00}^- + \sum_{nm} B_{klnm} b_{nm}^- \right) \Big/ A_{kl} \right] \tag{39}$$

to obtain improved values of the coefficients b_{ij}^-, and so forth [notice that a_{00}^- is known from Eq. (28)]. The coefficients a_{nm}^+ are then obtained from Eq. (31). Obviously, a reasonable first guess is $b_{nm}^- = 0$ since it implies that for $x < 0$ the distribution function is the Maxwellian

$$f^- = a_{00}^- \exp[-(\xi^- - V_0)^2 - (\eta^-)^2] \tag{40}$$

that is, the exact distribution function as $y^- \to -\infty$.

The main difficulty of solving Eqs. (39) and (31) resides in the evaluation of the coefficients B_{klnm} and E_{ijkl}. Though analytical expressions in terms of finite sums can be found for them,[27–29] they are so complicated that their use in the expressions (39) and (31) becomes numerically impracticable. However, the first guess $b_{nm}^- = 0$ is indeed a very good one. Its plausibility follows from the following arguments: apart from the term given by Eq. (40), the remaining members of the series (23) (notice that $a_{nm}^- = 0$ for $n, m \neq 0$) decay very rapidly to zero as $y^- \to -\infty$, since all the constants γ_{nm}^{0-} appearing in the exponentials are very large negative numbers (the smallest of them is $\gamma_{00}^{0-} = -2V_0$ of order $M^{-1/2}$). Moreover, any hydrodynamic description of the problem will necessarily yield f^- exactly through Eq. (40) because the heavy gas is in hypersonic conditions for

$x<0$ and does not "know" the presence of the light-gas shock until it reaches the discontinuity at $x=0$. Accordingly, for $x \leqslant 0$ heavy and light species are in equilibrium at temperature T_0 and velocity U_0.

A quantitative estimate of the errors of this approximation $b_{nm}^{-}=0$ may be obtained by inserting f^{-} of Eq. (40) and f^{+} given by the complete series (21) into the boundary condition (11) in order to determine the resulting coefficients a_{nm}^{+} and b_{nm}^{+}. Using the orthogonality properties of the functions G and Eqs. (A8)–(A9) of the Appendix, in addition to the recursion formula for the Hermite polynomials,[26] we obtain

$$\begin{aligned} a_{nm}^{+} 2^n n!\, (V+\gamma_{nm}^{+}) &= n_{p0}(m_p/2\pi kT)^{3/2} \exp[(V_0 - V)\,\gamma_{nm}^{+} \\ &\quad + (\gamma_{nm}^{+})^2(\theta^{-1}-3)/4]\,[(\theta-1)/\theta]^{n/2+m} \\ &\quad \times \{-[\theta(\theta-1)]^{-1/2} H_{n+1}(s_{nm})/2 \\ &\quad + [\theta^{1/2}(\theta-1)^{-1/2} s_{nm} + V + \gamma_{nm}^{+}]\, H_n(s_{nm})\} \end{aligned} \tag{41}$$

where the constants s_{nm} are

$$s_{nm} = [(V_0 - V)\,2\theta + \gamma_{nm}^{+}(1-2\theta)][\theta(\theta-1)]^{-1/2}/2 \tag{42}$$

with similar expressions for b_{nm}^{+}, but with γ_{nm}^{-} instead of γ_{nm}^{+}. From the equation for b_{nm}^{+} it follows that these coefficients are not exactly zero—as they should be in the exact solution—being instead of order $\exp(-1/M)$ (or smaller), which is a transcendentally small number for $M \ll 1$.[5] Considering that the inaccuracy of ignoring the finite width of the light-gas shock is far greater than $\exp(-1/M)$, an attempt of a more accurate description of the problem would make little physical sense. Therefore, with errors $O[\exp(-1/M)]$, the solution for $x>0$ can be written as (dropping the superscript $+$)

$$f = \sum_{nm} a_{nm} G_{nm}(\xi)\, L_m(\eta^2) \exp(-\eta^2 - \gamma_{nm}\, y) \tag{43}$$

[5] The dominant term in the coefficient b_{00}^{+} given by Eq. (41) with γ_{00}^{-} is the exponential term, which is not unity as in the case of a_{00}^{+}, because $\gamma_{00}^{-} = -2V$ instead of $\gamma_{00}^{+}=0$ [so that $a_{00}^{+}=O(1)$]. Therefore, $b_{00}^{+} \approx \exp[-2VV_0 - V^2(1-\theta^{-1})]$, where θ is always larger than one. V_0 is of order $M^{-1/2}$, and V, except for strong shocks, is of the same order (but for strong shocks, V_0 is much larger than $M^{-1/2}$). Then, $b_{00}^{+}=O[\exp(-1/M)]$. Numerical computations show that b_{nm}^{+} decreases very rapidly as n or m increase, so that all the coefficients b_{nm}^{+} are, at most, $O[\exp(-1/M)]$. Indeed, the same numerical computations show that the largest coefficient, that is, b_{00}^{+}, is much smaller than $\exp(-1/M)$. Thus, with $M_1=1.5$, for He–Ar $[\exp(-1/M)=4.54\times 10^{-5}]$, $b_{00}^{+}=1.12\times 10^{-7}$ and for He–Xe $[\exp(-1/M)=9.78\times 10^{-15}]$, $b_{00}^{+}=1.3\times 10^{-22}$.

with the coefficients a_{nm} given by Eq. (41). [Obviously, these coefficients a_{nm} are identical to those obtained from Eq. (31) by letting $b_{ij}^{-}=0$; also, the coefficient a_{00} given by Eq. (41) coincides with that of Eq. (27).] For $x<0$ the solution is the Maxwellian distribution (40), which, in terms of ξ and η, reads

$$f_0 = n_{p0}(m_p/2\pi kT_0)^{3/2} \exp[-\theta(\xi - V_0)^2 - \theta\eta^2] \tag{44}$$

where, for convenience, V_0 has been redefined as

$$V_0 = U_0(m_p/2kT)^{1/2} \tag{45}$$

[The parameter V_0 used in Eqs. (41) and (42) is also that defined by Eq. (45).]

3. RESULTS

Once the distribution function f is known, the evaluation of its moments is straightforward. Defining

$$n_p \equiv \int f\, d^3u \tag{46}$$

$$n_p \mathbf{U}_p \equiv \int \mathbf{u} f\, d^3u \tag{47}$$

$$\mathbf{P}_p \equiv m_p \int (\mathbf{u}-\mathbf{U}_p)(\mathbf{u}-\mathbf{U}_p)\, f\, d^3u \tag{48}$$

$$\mathbf{T}_p \equiv \mathbf{P}_p/n_p k \tag{49}$$

$$\mathbf{Q}_p \equiv m_p \int (\mathbf{u}-\mathbf{U}_p)(\mathbf{u}-\mathbf{U}_p)(\mathbf{u}-\mathbf{U}_p)\, f\, d^3u \tag{50}$$

$$d_{nm} \equiv (a_{nm}/n_{p0})(2\pi kT/m_p)^{3/2} \tag{51}$$

and making use of the orthogonality properties described in the Appendix, we obtain the following expressions for the dimensionless density, mean velocity, temperature tensor, and heat flux tensor:

$$N_p \equiv n_p/n_{p0} = \sum_{n=0}^{\infty} d_{n0}(-\gamma_{n0})^n \exp(-\gamma_{n0}\, y) \tag{52}$$

$$U_p \equiv U_{px}(m_p/2kT)^{1/2} = V_0/N_p \tag{53}$$

$$\begin{aligned} T_{p\parallel} &\equiv P_{pxx}/n_p k T_0 \\ &= (2\theta/N_p)\left\{ d_{00}(V^2+1/2) \right. \\ &\quad \left. + \sum_{n=1}^{\infty} [d_{n0}(-\gamma_{n0})^n \exp(-\gamma_{n0}\, y)(1/2 - n/\gamma_{n0}^2)] - V_0^2/N_p \right\} \end{aligned} \tag{54}$$

$$
\begin{aligned}
T_{p\perp} &\equiv P_{pyy}/n_p kT_0 \\
&= P_{pzz}/n_p kT_0 \\
&= (\theta/N_p)\Big\{d_{00} - d_{01}\exp(-\gamma_{01}\,y) \\
&\quad + \sum_{n=1}^{\infty}\left[d_{n0}(-\gamma_{n0})^n \exp(-\gamma_{n0}\,y) - d_{n1}(-\gamma_{n1})^n \exp(-\gamma_{n1}\,y)\right]\Big\}
\end{aligned} \tag{55}
$$

$$
\begin{aligned}
Q_{p||} &\equiv Q_{pxxx}/U_{px}P_{pxx} \\
&= (2\theta/V_0 T_{p||})\Big\{d_{00}(V^2+3/2)\,V \\
&\quad - \sum_{n=1}^{\infty}\left[d_{n0}(-\gamma_{n0})^n \exp(-\gamma_{n0}\,y)(2n/\gamma_{n0}^3)\right]\Big\} - 3 - 2\theta V_0^2/T_{p||}N_p^2
\end{aligned} \tag{56}
$$

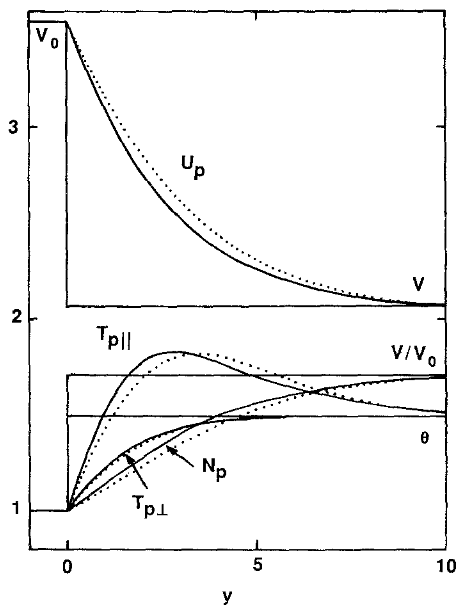

Fig. 1. Plots of N_p, U_p, $T_{p||}$, and $T_{p\perp}$ for He–Ar with $M_1 = 1.5$. The horizontal straight lines are the pre- and post-shock values of these properties for the light gas (as explained in the text, the light-gas shock wave is a discontinuity occurring at $y = 0$). The dotted lines correspond to the solution of the hypersonic approximation (60)–(63).

$$Q_{p\perp} \equiv Q_{pxyy}/U_{px}P_{pyy}$$
$$= Q_{pxzz}/U_{px}P_{pzz}$$
$$= (\theta/V_0 T_{p\perp}) \left\{ d_{00} V - \sum_{n=1}^{\infty} [2d_{n1}(-\gamma_{n1})^n \exp(-\gamma_{n1} y)/\gamma_{n1}] \right\} - 1 \quad (57)$$

All the remaining terms of $\mathbf{T}_p$ and $\mathbf{Q}_p$ are equal to zero.

These moments of f for $x > 0$ are shown in Figs. 1–3 for He–Ar and He–Xe mixtures ($M = 0.10$ and $M = 0.031$, respectively) with Mach number $M_1 = 1.5$.

Some comments on the numerical computations are worth mentioning here. The convergence of the series (52)–(57) is rather slow (particularly near $y = 0$), the more so the larger the Mach number. Thus, for He–Xe, to reach $N_p(y = 0) = 1$ with an error less than or equal than 10^{-4}, 16 terms of the series (52) were needed for $M_1 = 1.5$; 40 terms for $M_1 = 2$; 141 terms for $M_1 = 3$; etc. The results of Figs. 1–3 for $M_1 = 1.5$ were calculated with a number of terms in the series (52)–(57) such that $N_p(y = 0) - 1$ is less than 10^{-9} (of course, double precision was used in the numerical computations). For moderately large values of M_1, the use of logarithms was required in

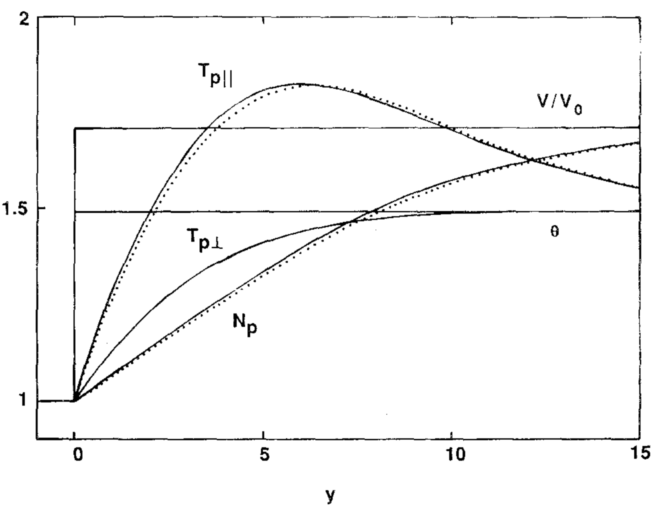

Fig. 2. Plots of N_p, $T_{p\|}$, and $T_{p\perp}$ for He–Xe with $M_1 = 1.5$. The dotted lines correspond to the solution of the hypersonic approximation (60)–(63) [$T_{p\perp}$ given by the hypersonic approximation is indistinguishable from $T_{p\perp}$ given by Eq. (55)].

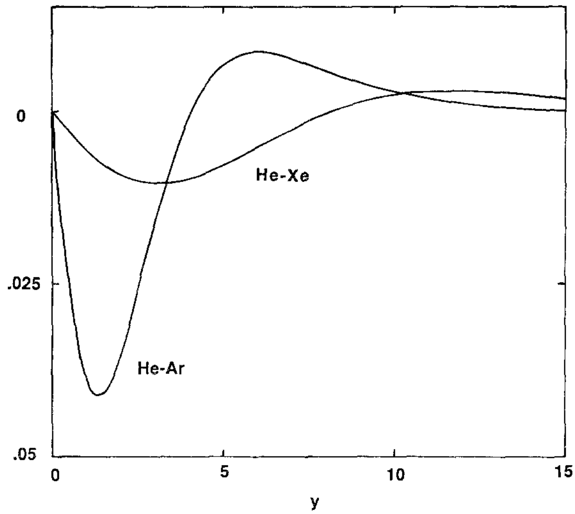

Fig. 3. Heat flux $Q_{p\|}$ [Eq. (56)] for He–Xe and He–Ar with $M_1 = 1.5$.

order to avoid numerical overflows in the computer when evaluating the large-n terms in the series (52)–(57). To this end, it is preferable to compute the Hermite polynomials in terms of the Laguerre polynomials:[26]

$$H_{2m}(x) = (-1)^m \, 2^{2m} m! \, L_m^{(-1/2)}(x^2) \tag{58}$$

$$H_{2m+1}(x) = (-1)^m \, 2^{2m+1} m! \, x L_m^{(1/2)}(x^2), \qquad m = 0, 1, 2,... \tag{59}$$

As a comparison, Figs. 1 and 2 also show the results from the lowest order hypersonic approximation,[23–25] in which $\mathbf{P}_p$ is neglected in the momentum conservation equation and $\mathbf{Q}_p$ is ignored in the equation for the temperature tensor. Within these assumptions, N_p, U_p, $T_{p\|}$, and $T_{p\perp}$ obey the equations

$$N_p U_p = V_0 \tag{60}$$

$$dU_p/dy = V/U_p - 1 \tag{61}$$

$$dT_{p\|}/dy = 2(\theta - T_{p\|} V/U_p)/U_p \tag{62}$$

$$dT_{p\perp}/dy = 2(\theta - T_{p\perp})/U_p \tag{63}$$

with the boundary conditions at $y = 0$: $N_p = 1$, $U_p = V_0 = M_1(\gamma/2M\theta)^{1/2}$, $T_{p\|} = T_{p\perp} = 1$. Obviously, the agreement between these hypersonic results and those of Eqs. (52)–(55) is much better for He–Xe than for He–Ar, since

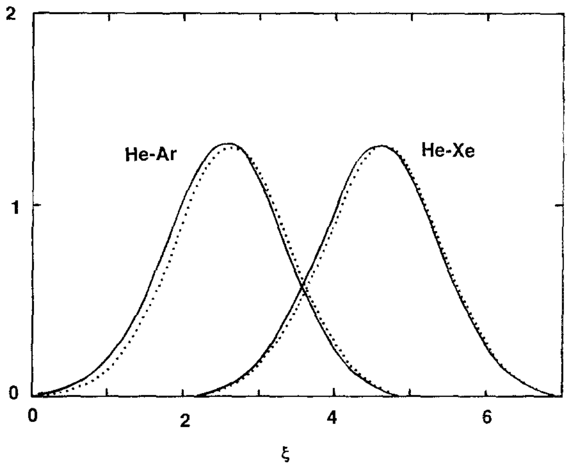

Fig. 4. Section $\eta = 0$ of the distribution function given by Eq. (43) [divided by $n_{p0}(2\pi kT/m_p)^{-3/2}$] for He–Ar (at $y = 3$) and He–Xe (at $y = 6$) with $M_1 = 1.5$. The dotted lines correspond to the Gaussian distribution (64).

the hypersonic approximation is the better, the smaller the mass ratio M is. As shown in Ref. 25, the errors of the results given by Eqs. (60)–(63) (the lowest order of the hypersonic expansion) are $O(M)$, while the errors of the solution (52)–(57) are by far much smaller [of order $\exp(-1/M)$].

Finally, the distribution function (43) [after making it dimensionless with $n_{p0}(2\pi kT/m_p)^{-3/2}$ and evaluated at $\eta = 0$] is shown in Fig. 4 for the same cases as in Figs. 1–3. In addition, the same figure contains the Gaussian distribution

$$f_G = (N_p \theta^{3/2}/T_{p\|}^{1/2} T_{p\perp}) \exp\{-\theta[(\xi - U_p)^2/T_{p\|} + \eta^2/T_{p\perp}]\} \qquad (64)$$

with N_p, U_p, $T_{p\|}$, and $T_{p\perp}$ given by the hypersonic approximation (60)–(63). As shown in Ref. 25, this Gaussian distribution is the lowest order solution of a hypersonic expansion of the FP equation. Notice that the heat fluxes (Fig. 3) are very small, but they are not exactly zero as would correspond to a Gaussian distribution. The values of y for the distribution functions plotted in Fig. 4 have been chosen as $y = 3$ (He–Ar) and $y = 6$ (He–Xe), where, approximately, the parallel temperature $T_{p\|}$ reaches a maximum so that the conditions are far removed from equilibrium and the FP and the hypersonic solutions differ most (see Figs. 1 and 2).

APPENDIX. ORTHOGONALITY PROPERTIES AND OTHER RELATIONS

The functions $G^{\pm}_{nm}$ and $G^{0\pm}_{nm}$ [Eqs. (29)–(30)] satisfy the ordinary differential equations

$$d[\exp(\xi - V)^2\, dG^{\pm}_{nm}/d\xi]/d\xi + 2(\gamma^{\pm}_{nm}\xi + 1 - 2m)\exp(\xi - V)^2\, G^{\pm}_{nm} = 0 \qquad \text{(A1)}$$

and similarly for $G^{0\pm}_{nm}$ with V_0 and $\gamma^{0\pm}_{nm}$. Hence, the orthogonality properties are

$$\int_{-\infty}^{+\infty} d\xi\ \xi G^{\pm}_{n'm} G^{\pm}_{nm} \exp(\xi - V)^2 = 0, \qquad \text{if} \quad n \neq n' \qquad \text{(A2)}$$

with identical expression for $G^{0\pm}_{nm}$, where V is substituted by V_0. For $n = n'$ the value of the integral (A2) is

$$n!\, 2^n \pi^{1/2}(V + \gamma^{\pm}_{nm}) \exp[(\gamma^{\pm}_{nm})^2/2]$$

Since $G^{+}_{00} = \exp[-(\xi - V)^2]$, we have

$$\begin{aligned} \int_{-\infty}^{+\infty} d\xi\ \xi G^{+}_{n0} &= 0, \qquad && n \neq 0 \\ &= \pi^{1/2} V, && n = 0 \end{aligned} \qquad \text{(A3)}$$

For any value of the integers n and m, since[30]

$$\begin{aligned} &\int_{-\infty}^{+\infty} dx \exp(-x^2)\, H_m(x + y)\, H_n(x + z) \\ &\quad = \sqrt{\pi}\, m!\, 2^n z^{n-m} L_m^{(n-m)}(-2yz), \qquad m \leqslant n \end{aligned} \qquad \text{(A4)}$$

where $L_m^{(n-m)}(x)$ are Laguerre polynomials, one obtains, on using $L_1^{(a)}(x) = -x + a + 1$ and Eq. (20),

$$\begin{aligned} \int_{-\infty}^{+\infty} d\xi\ \xi G^{\pm}_{nm} &= -2\sqrt{\pi}\, m(-\gamma^{\pm}_{nm})^{n-1}, \qquad && n \neq 0 \\ &= \sqrt{\pi}(V + \gamma^{\pm}_{0m}/2), && n = 0 \end{aligned} \qquad \text{(A5)}$$

and

$$\int_{-\infty}^{+\infty} d\xi\ G^{\pm}_{nm} = \sqrt{\pi}(-\gamma^{\pm}_{nm})^n \qquad \text{(A6)}$$

Equations equivalent to (A5) and (A6) would apply to $G^{0\pm}_{nm}$ after substituting $\gamma^{\pm}_{nm}$ and V by $\gamma^{0\pm}_{nm}$ and V_0.

The orthogonality properties of the Laguerre polynomials can be written as[26]

$$\int_0^{+\infty} dx\, L_m(x)\, L_{m'}(x) \exp(-x) = 0, \qquad m \neq m' \\ = 1, \qquad m = m' \tag{A7}$$

Other integrals used to evaluate the coefficients a_{nm} are[30],[31]

$$\int_{-\infty}^{+\infty} dx \exp\left[-\frac{(x-y)^2}{a^2}\right] H_m(x)\, H_n(x) \tag{A8}$$

$$= a\sqrt{\pi} \sum_{k=0}^{\min(n,m)} k! \binom{m}{k}\binom{n}{k} (1-a^2)^{(m+n)/2-k}\, 2^k H_{m+n-2k}\left[\frac{y}{(1-a)^{1/2}}\right]$$

$$\int_0^{+\infty} dx \exp(-\theta x)\, L_m(x) = [(\theta-1)/\theta]^m/\theta \tag{A9}$$

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