The Milne problem: A study of the mass dependence

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(Received 28 July 1981; revised manuscript received 30 March 1982)

The Milne problem is considered with the Boltzmann equation without approximation to the collision operator. The general solution is given as the sum of spatial transient and asymptotic functions. Solutions of the Boltzmann equation with a hard-sphere cross section are obtained by expansions in Burnett functions. Convergence of the distribution function and associated quantities, such as spatial eigenvalues, extrapolation length, diffusion coefficient, and density profile is studied. It is found that convergence can be achieved with the expansion in Burnett functions. In particular, the importance of retaining a large number of polynomials in angle is demonstrated. The dependence of the solution and associated quantities on the mass ratio $\gamma=m_1/m$ is examined, where m_1 and m are the mass of medium and test particles, respectively. Wherever possible, comparison with the results of previous researchers is given.

I. INTRODUCTION

The Milne problem investigated in this paper concerns the stationary velocity distribution of an ensemble of test particles dilutely dispersed in a medium or moderator composed of a different constituent that acts as a constant-temperature heat bath. The medium occupies the half space $r>0$, whereas a vacuum exists in the half space $r\leq 0$. Figure 1 shows the physical problem that we are considering. A current density of magnitude $\bar{j}$, directed in the negative r direction, exists in the medium. In the present work, it is further assumed that there is no absorption nor other sources of particles, although these assumptions are not crucial to the development. The problem consists of determining the steady distribution of test particles and, in particular, the angular distribution of these particles emerging from the medium into the vacuum at $r=0$.

This problem is a fundamental problem in physics and has application to radiation-transfer problems,[1] neutron-transport theory,[2-5] and rarefied-gas dynamics.[2,6,7] In the astrophysical context, the test particles are photons and the quantities of interest are the steady intensity of radiation in the interior of a star and the emergent angular distribution. This is the problem originally considered by Milne.[8] For neutron transport, the test particles are neutrons diffusing through a reactor and the steady neutron velocity distribution is the desired quantity. In this case, an important variable is the mass ratio $\gamma=m_1/m$, where m_1 and m are the masses of the medium and the test particles, respectively. The relationship between the neutron-transport and radiative-transport problems has been presented in considerable detail elsewhere.[1-3] It is important to mention, however, that for $\gamma=\infty$ (the one-speed case or Lorentz limit), the neutron-transport problem becomes identical with the radiative-transfer problem (the restricted Milne problem in the gray case[1,9]). This special case is usually what is meant by the Milne problem for which an exact solution exists.[10]

The present paper considers the Milne problem as a kinetic-theory problem in rarefied-gas dynamics. The basic objective is to obtain converged solutions of the Boltzmann equation subject to the boundary condition that there are no test particles incident on

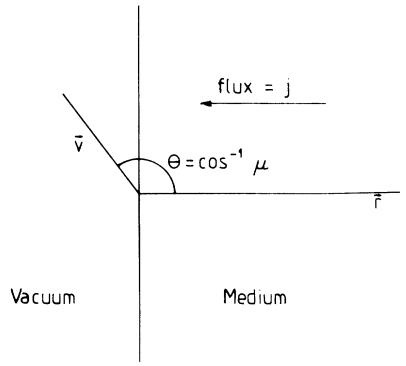

FIG. 1. Geometry of the Milne problem.

the medium from the vacuum. The velocity-distribution function is sought for a wide range of values of the mass ratio γ. The basic assumptions are that only test particle-heat-bath collisions need be considered and that the differential cross section σ is a hard-sphere cross section, that is, $\sigma=\frac{1}{4}d^2$, where d is the average of the diameters of the two species. Important macroscopic quantities such as the number density profile $\bar{n}(r)$ and the diffusion coefficient $\bar{D}$ are calculated.

From the viewpoint of rarefied-gas dynamics, the important aspect of the problem is the effects that occur within several mean-free paths of the boundary at $r=0$. To simplify the discussion in the remainder of this Introduction, the bath particle density $\bar{n}_1$ will be assumed constant. (In Sec. II, it is shown how this assumption may be relaxed.) Far from the boundary, in the positive r direction, hydrodynamic equations are valid, which for the present work is the diffusion equation

$$\bar{j}=-\bar{D}\frac{d\bar{n}^{\rm as}(r)}{dr}\ , \tag{1.1}$$

which relates the diffusion flux $\bar{j}$ and the gradient of the asymptotic $(r\to\infty)$ density profile $\bar{n}^{\rm as}(r)$. However, one finds that the asymptotic density extrapolates to zero at the point $r=-\bar{q}$, where $\bar{q}$ is referred to as the extrapolation length. Consequently, Eq. (1.1) is not valid near the boundary at $r=0$. The calculation of the density profile and the extrapolation length is one of the objectives of the present work.

In the Lorentz limit $(\gamma=\infty)$, the Boltzmann equation reduces to the simpler one-speed version for which an analytic solution exists[10] and $\bar{q}$ is given as a definite integral whose numerical value is $0.710\,45l(\infty)$, where

$$l(\infty)=(n_1\pi d^2)^{-1}\ .$$

Very little work has been done with the full Boltzmann collision operator and the variation with mass ratio has received little attention. Conkie,[11] and later Kladnik and Kuscer[12] considered the case of equal masses $(\gamma=1)$ and obtained the values $0.763l(\infty)$ and $0.935l(\infty)$, respectively. (The present work confirms that the result obtained by Conkie is in error as suggested earlier by Kladnik and Kuscer.) Williams[13] and later Arkuszewski[14] approximated the Boltzmann collision operator with a separable kernel and obtained analytic solutions for all values of γ. They found that $\bar{q}$ decreases with decreasing γ from the one-speed value to the value $\bar{q}=0.538l(\infty)$ for $\gamma=1$. This mass dependence differs from that inferred from the results by Kladnik and Kuscer[12] which suggest that $\bar{q}$ increases with decreasing γ.

The present paper considers solutions of the Boltzmann equation without modification to the collision operator. The distribution function is written as a sum of spatial transient and asymptotic parts.[2] The spatial transient portion of the solution plays an important role near the boundary, whereas the asymptotic solution dominates in the region far from the boundary. An expansion in Burnett functions is employed following the procedure introduced by Frankowski *et al.*[15] in their study of heat conduction in a rarefied medium. We demonstrate, in the application to the Milne problem, that this expansion method does give convergent solutions. The method permits the study of the variation of the distribution function, density profile, and extrapolation length with mass ratio γ.

There are several other methods of solution of the Boltzmann equation that can be used in the study of the Milne problem. In particular, there exist variational methods,[12,16–19] discrete ordinate methods,[20–23] and other types of expansion procedures.[2,24] Each method has distinct advantages and disadvantages and we will not attempt a comprehensive comparison here. The expansion procedure used in the present work was employed since the matrix elements of the Boltzmann collision operator with the Burnett functions have been previously calculated.[25] It is not known whether the matrix elements for other basis functions, such as half-ranged polynomials, can be as easily determined. Variational procedures with simple trial functions do give very good initial estimates of quantities such as the extrapolation length. However, more accurate results with more complicated variational functions are not as easily obtained. The discrete ordinate method has been used in only a few cases and it is diffucult to judge how flexible it may be in its application to a variety of different problems.

The present methods should be useful in the study of a wide variety of gas dynamical problems. These include, for example, the Kramers,[18] Couette,[19] Poiseuille,[19] and temperature slip problems.[2,7,15] The mathematical methods common to these problems and to neutron-transport theory have been emphasized by several authors.[2–7] The present authors' work in the Milne problem stems from an interest in the thermal escape of particles from a planetary atmosphere.[26,27] This problem is somewhat similar to the Milne problem but has an additional complication in that test particles escape

from the atmosphere if their speed exceeds the escape speed. Consequently, the point of departure of the planetary escape problem from the Milne problem is in the nature of the boundary condition. It is anticipated that the present methods of solution of the Boltzmann equation will prove useful in the planetary escape problem. In particular, the hard-sphere model employed in this work was shown to be appropriate to the escape problem.[28]

The present paper on the Milne problem is organized as follows: Section II contains a discussion of the Boltzmann equation for the problem and the division of the solution into spatial transient and asymptotic portions. The way in which the boundary condition specifies a unique solution is described in Sec. III. The numerical results obtained appear in Sec. IV. A discussion is given in Sec. V.

II. FORM AND PROPERTIES OF THE GENERAL SOLUTION

For steady-state conditions the Boltzmann equation for the velocity-distribution function of test particles $\bar{f}(r,v,\mu)$ is

$$v\mu\frac{\partial}{\partial r}\bar{f}(r,v,\mu)=\bar{n}_1(r)\bar{J}(\bar{f}(r,v,\mu)) , \tag{2.1}$$

where $\mu=\cos\theta$ and θ is the angle between $\vec{v}$ and the positive r axis as shown in Fig. 1. In Eq. (2.1), $\bar{n}_1(r)$ is the number density of the scattering medium and the Boltzmann collision operator $\bar{J}$ is defined by[29,30]

$$\bar{J}(\bar{f}(r,\vec{v}))=\int\int[\bar{f}_1^M(v_1')\bar{f}(r,\vec{v}')-\bar{f}_1^M(v_1)\bar{f}(r,\vec{v})] \times\sigma(g,\Omega)g\,d\Omega\,d\vec{v}_1 . \tag{2.2}$$

The notation in this paper is that of kinetic theory rather than of neutron transport.

In Eq. (2.2), $\vec{g}=\vec{v}-\vec{v}_1$ is the relative velocity, σ is the differential cross section, Ω is the scattering solid angle, and $\bar{f}_1^M$ is the Maxwellian distribution given by

$$\bar{f}_1^M(v_1)=(m_1/2\pi kT_1)^{3/2}\exp(-m_1v_1^2/2kT_1) , \tag{2.3}$$

where k is Boltzmann's constant and T_1 is the bath temperature. Primes in Eq. (2.2) refer to post-collision velocities. The cross section in Eq. (2.2) will be taken to be the hard-sphere cross section.

It is convenient to employ, instead of r, the dimensionless spatial variable, analogous to an optical depth,[1,2] defined by

$$x=\pi d^2\int_0^r\bar{n}_1(r')dr' . \tag{2.4}$$

With this change of variable, the Boltzmann equation can be written in the form

$$p\mu\frac{\partial}{\partial x}f(x,p,\mu)=J(f(x,p,\mu)) , \tag{2.5}$$

where $J=\bar{J}/(\pi d^2v_0)$, $f=\bar{f}[v_0/\bar{n}_1(r)\pi d^2]^3$, $v_0^2=2kT_1/m$, and $p=v/v_0$.

In the Lorentz limit (or one-speed case), when the medium particles become infinitely heavy, the Boltzmann collision operator $\bar{J}$ reduces to the Lorentz operator, that is,

$$\bar{J}(\bar{f}(\vec{v}))\underset{\gamma\to\infty}{\to}\tfrac{1}{4}d^2v\int[\bar{f}(\vec{v}')-\bar{f}(\vec{v})]d\Omega .$$

For this case, one has the simpler one-speed transport equation

$$\mu\frac{\partial f}{\partial x}(x,\mu)=\tfrac{1}{2}\int_{-1}^{1}f(x,\mu')d\mu'-f(x,\mu) , \tag{2.6}$$

which is identical to the radiative-transfer equation in the gray case.[1]

In the present paper, we seek solutions to the more general equation, Eq. (2.5), subject to the boundary condition at $x=0$,

$$f(0,p,\mu)=0,\quad 0<\mu<1 \tag{2.7}$$

since it is assumed that no particles in the vacuum return to the medium. A more detailed discussion of boundary conditions is presented in Sec. III.

The general solution is written as the sum of a spatial transient part $f^{\rm tr}$ and an asymptotic part $f^{\rm as}$, that is,

$$f=f^{\rm tr}+f^{\rm as} . \tag{2.8}$$

The transient solution plays an important role in the region near $x=0$ and decays out in a distance of the order of several mean-free paths. The asymptotic solution dominates at large distances from the boundary, where hydrodynamics is valid. The separation of the solution in this way has been discussed by Williams[2] in connection with several other similar problems.

A. Spatial transient solution

The transient solution is written in the form

$$f^{\rm tr}(x,p,\mu)=\sum_{k=1}^{\infty}a_ke^{g_kx}R_k(p,\mu) , \tag{2.9}$$

which, when substituted into Eq. (2.5), yields

$$J(R_k(p,\mu))=(p\mu)g_k R_k(p,\mu) . \tag{2.10}$$

Equation (2.10) is in the form of an eigenvalue equation for the operator $(p\mu)^{-1}J$, with eigenfunctions $R_k(p,\mu)$ and spatial eigenvalues g_k. The expansion coefficients a_k are determined by the boundary conditions as discussed in Sec. III. The transient solution is chosen in this form so that $f^{\rm tr}\rightarrow 0$ as $x\rightarrow\infty$. Obviously, this requires that only negative eigenvalues g_k be included in Eq. (2.9).

The eigenfunctions R_k and corresponding eigenvalues g_k are determined by an expansion in Burnett functions $\psi_{nl}(p,\mu)$,

$$R_k(p,\mu)=f^M(p)\sum_{n=0}^{\infty}\sum_{l=0}^{\infty} b_{nl}^k\psi_{nl}(p,\mu) , \tag{2.11}$$

where $f^M(p)=\pi^{-3/2}e^{-p^2}$ and

$$\psi_{nl}(p,\mu)=N_{nl}p^l L_n^{l+1/2}(p^2)P_l(\mu) . \tag{2.12}$$

In Eq. (2.12), P_l are the Legendre polynomials and $L_n^{l+1/2}(p^2)$ are the associated Laguerre polynomials defined by

$$L_n^{l+1/2}(p^2)=\sum_{m=0}^{n}\frac{(-1)^m\Gamma(n+l+\frac{3}{2})}{m!\Gamma(m+l+\frac{3}{2})(n-m)!}p^{2m} . \tag{2.13}$$

The normalization factors N_{nl} are chosen such that the norm

$$\begin{aligned}(\psi_{nl},\psi_{n'l'})&=\pi^{-3/2}\int e^{-p^2}\psi_{nl}(\vec{\rm p})\psi_{n'l'}(\vec{\rm p})d\vec{\rm p} ,\\ &=\delta_{nn'}\delta_{ll'} .\end{aligned} \tag{2.14}$$

Equations (2.12)–(2.14) yield the result

$$N_{nl}=[\sqrt{\pi}n!(2l+1)/2\Gamma(n+l+\tfrac{3}{2})]^{1/2} . \tag{2.15}$$

A solution to Eq. (2.10) is obtained with the substitution of the expansion equation (2.11) into Eq. (2.10), multiplication by each basis function, and integration over $\vec{\rm p}$. This procedure converts Eq. (2.10) into an infinite set of linear equations

$$\sum_{n'=0}^{\infty}\sum_{l'=0}^{\infty}(A_{nl,n'l'}-g_k B_{nl,n'l'})b_{n'l'}^k=0 , \tag{2.16}$$

where $A_{nl,n'l'}$ are the matrix elements of the Boltzmann collision operator calculated by the authors in an earlier paper.[25] In order to make connection with this previous calculation, it is convenient to define the collision operator

$$\begin{aligned}\bar{I}(h(\vec{\rm v}))&=(\bar{f}^M(v))^{-1}\bar{J}(\bar{f}^M(v)h(\vec{\rm v}))\\ &=\int\int\bar{f}_1^M(v_1)[h(\vec{\rm v}')-h(\vec{\rm v})]\\ &\quad\times\sigma(g,\Omega)g\,d\Omega\,d\vec{\rm v}_1 ,\end{aligned} \tag{2.17}$$

and the corresponding dimensionless operator $I=\bar{I}/(\pi d^2 v_0)$. In terms of I, we see that

$$A_{nl,n'l'}=(\psi_{nl},I\psi_{n'l'}) , \tag{2.18}$$

$$B_{nl,n'l'}=(\psi_{nl},p\mu\psi_{n'l'}) . \tag{2.19}$$

The matrix $A_{nl,n'l'}$ can be obtained by multiplying $M_{lnn'}^{(1)}$ in Eq. (25) of Ref. 25 by the factor

$$\delta_{ll'}N_{nl}N_{n'l}[4\pi/(2l+1)](\pi d^2 v_0)^{-1} .$$

The matrix elements of the right-hand side of Eq. (2.10), $B_{nl,n'l'}$, are readily evaluated using the recursion relations for the Legendre and Laguerre polynomials. The result is

$$B_{nl,n'l'}=\begin{cases}(l+1)[(n+l+\frac{3}{2})/(2l+1)(2l+3)]^{1/2}, & n'=n,\ l'=l+1\\ -(l+1)[n/(2l+1)(2l+3)]^{1/2}, & n'=n-1,\ l'=l+1\\ l[(n+l+\frac{1}{2})/(2l-1)(2l+1)]^{1/2}, & n'=n,\ l'=l-1\\ -l[(n+1)/(2l-1)(2l+1)]^{1/2}, & n'=n+1,\ l'=l+1\\ 0, \quad \text{otherwise} .\end{cases} \tag{2.20}$$

Approximate eigenfunctions and eigenvalues are obtained by truncation of the summations in Eq. (2.16) at $n'=N$ and $l'=L$ which yields $K=(N+1)(L+1)$ linear homogeneous equations in K unknowns. A solution exists if and only if the determinant of the matrix in square brackets is zero. The solution of the resulting secular equation gives approximate values for the first K eigenvalues g_k.

The work here is similar to the procedure by Frankowski *et al.*[15] in their study of heat conduction, although they chose to divide through by $p\mu$

in Eq. (2.10) and then take matrix elements. An important feature of the eigenvalue spectrum, as shown by Frankowksi *et al.*,[15] is that the exact eigenvalues g_k occur in positive and negative pairs. Likewise, the zero eigenvalue is doubly degenerate. For finite orders, this pairing may be shown by splitting Eq. (2.16) into groups for even and odd l. Elimination of one group in favor of the other yields an eigenvalue equation for g_k^2. This result occurs provided the dimension of the even and odd submatrices are equal or equivalently if L is odd.

Since a necessary condition for the transient solution is that it vanish as $x \to \infty$, zero and positive eigenvalues must be excluded from Eq. (2.9). Consequently, $a_k = 0$ for $g_k \geq 0$ and the transient solution is now written in the form

$$f^{\rm tr}(x,p,\mu) = \sum_{k=1}^{1/2K-1} a_k e^{g_k x} R_k(p,\mu) , \tag{2.21}$$

where the sum extends only over negative g_k.

The present procedure is also somewhat similar to that employed by Conkie[11] in his study of this problem for $\gamma = 1$. However, his choice of basis functions for the expansion of $R_k(p,\mu)$ differs from ours [Eqs. (2.11)–(2.13)] and the corresponding matrix elements had to be evaluated numerically.

B. Asymptotic solution

The asymptotic solution, following the work by Kladnik and Kuscer,[12] is chosen to be of the form

$$f^{\rm as}(x,p,\mu) = -(j/D) f^M(p)[q + x - \mu U(p)] , \tag{2.22}$$

where $j = \bar{j}/v_0[\bar{n}_1(r)\pi d^2]^3$ and $D = \bar{D}/[v_0/\bar{n}_1(r)\pi d^2]$ are the dimensionless flux and diffusion coefficient, respectively. These are defined by

$$j = \int f(x,p,\mu) p\mu \, d\vec{\rm p} \tag{2.23}$$

and

$$D = \int f^M(p) p\mu^2 U(p) d\vec{\rm p} , \tag{2.24}$$

where Eq. (2.22) has been used. The choice of Eq. (2.22) for the solution far from the boundary can be appreciated by considering the contribution it makes to the density. Integration of Eq. (2.22) yields

$$n^{\rm as}(x) = \int f^{\rm as}(x,p,\mu) d\vec{\rm p} = -(j/D)(q + x) , \tag{2.25}$$

where the term proportional to μ in Eq. (2.22) does not contribute. This density profile satisfies the diffusion equation

$$j = -D \frac{dn^{\rm as}}{dx} \tag{2.26}$$

and extrapolates to zero at $x = -q$. It is also important to note that the transient solution $f^{\rm tr}$ does not contribute to j.

Substitution of Eq. (2.22) into Eq. (2.5) yields the following integral equation for the function $U(p)$:

$$I(\mu U(p)) = -p\mu . \tag{2.27}$$

The function $U(p)$ is determined by its expansion in Laguerre polynomials; that is,

$$U(p) = \sum_{n'=0}^{\infty} d_{n'} N_{n'1} p L_{n'}^{3/2}(p^2) , \tag{2.28}$$

or in terms of the Burnett functions of Eq. (2.12),

$$\mu U(p) = \sum_{n'=0}^{\infty} d_{n'} \psi_{n'1}(p,\mu) . \tag{2.29}$$

With Eq. (2.29) in Eq. (2.27) and taking matrix elements, we obtain,

$$\sum_{n'=0}^{\infty} A_{n1,n'1} d_{n'} = -\delta_{n0}/\sqrt{2} . \tag{2.30}$$

With Eqs. (2.26) and (2.29), it is easily seen that the diffusion coefficient is given by

$$D = d_0/\sqrt{2} . \tag{2.31}$$

An approximate solution is obtained with the truncation of the expansion at $n' = N$ and inversion of the resulting finite set of equations. This yields a set of N-expansion coefficients and an estimate for the diffusion coefficient. The foregoing will be recognized as the usual procedure for the calculation of the diffusion coefficient with the Chapman-Enskog scheme.[29,30]

C. General solution

An important feature of Eq. (2.5) is that when integrated over $\vec{\rm p}$, the right-hand side vanishes due to particle conservation with the result that

$$\int p\mu \frac{\partial f}{\partial x} d\vec{\rm p} = 0 .$$

In view of the definition of the flux j, Eq. (2.23), this result indicates that $dj/dx = 0$ and, therefore,

that j is constant. Furthermore, since the kinetic equation and associated boundary conditions (Sec. III) are homogeneous, some normalization of the distribution function is required. This normalization is fixed, as is usually done,[11-14] by setting $j=-1$.

With this choice, the general solution is with Eqs. (2.9), (2.11), (2.21), and (2.22) given by

$$f(x,p,\mu)=f^M(p)\left[\sum_{k=1}^{1/2K-1} a_k e^{g_k x}\sum_{l=0}^{L}\sum_{n=0}^{N} b_{nl}^k \psi_{nl}(p,\mu)+D^{-1}\left[q+x-\sum_{n=1}^{N} d_n\psi_{nl}(p,\mu)\right]\right] . \tag{2.32}$$

The coefficients b_{nl}^k in Eq. (2.32) are determined with Eq. (2.16). Similarly, the d_n coefficients and the diffusion coefficient are calculated with Eqs. (2.30) and (2.31), respectively. In order for $f(x,p,\mu)$ in Eq. (2.32) to be completely specified, the $(\frac{1}{2}K-1)a_k$ coefficients and the extrapolation length must be determined. These $\frac{1}{2}K$ quantities are fixed by the boundary conditions.

III. BOUNDARY CONDITIONS

It is impossible for a finite expansion such as Eq. (2.32) to satisfy the boundary condition Eq. (2.7) for all p and all $\mu>0$. As a result, there is no *a priori* preferred method to determine the remaining $\frac{1}{2}K$ quantities. In the present work, three methods are employed. These include the Marshak and Mark methods employed in neutron-transport theory,[3-5] and a third method based on a variational principle.

In the Mark method, the distribution function at $x=0$ is set to zero at $(N+1)$ p_ν points and $(L+1)/2$ μ_λ points corresponding to incoming directions, in accordance with Eq. (2.7). For the large orders, N and L, used in the present work, large instabilities occurred with this method and the Mark method was abandoned. No detailed study was made to ascertain the source of the difficulty.

A. Marshak boundary condition

The Marshak boundary conditions[3-5] set to zero various moments of the distribution function at $x=0$;

$$\int H(\mu)\psi_{nl}(p,\mu)f(0,p,\mu)d\vec{\mathrm{p}}=0 . \tag{3.1}$$

In Eq. (3.1), $H(\mu)$ is the Heaviside function, that is, $H=1$ for $\mu\geq 0$ and $H=0$ for $\mu<0$. The usual procedure is to employ Eq. (3.1) for all n but only for odd l which then gives the required $K/2$ conditions.

With Eq. (2.32) in Eq. (3.1), we obtain

$$\sum_{k=1}^{1/2K-1} a_k \sum_{n'=0}^{N}\sum_{l'=0}^{L} b_{n'l'}^k G_{nl,n'l'} + D^{-1}\left[qG_{nl,00}-\sum_{n'=0}^{N} d_{n'}G_{nl,n'1}\right]=0 , \tag{3.2}$$

where

$$G_{nl,n'l'}=\int H(\mu)\psi_{nl}(p,\mu)\psi_{n'l'}(p,\mu)d\vec{\mathrm{p}} . \tag{3.3}$$

An explicit expression for these quantities can be derived with the expansion Eq. (2.4). The method of evaluation essentially follows the calculation of Frankowski *et al.*[15] The details of this calculation can be obtained by writing to the authors. In particular, it can be shown that

$$G_{nl,n'1}=\tfrac{1}{2}\delta_{l1}\delta_{nn'} . \tag{3.4}$$

With Eq. (3.4) and the definition

$$W_{nl}^k=\sum_{n'=0}^{N}\sum_{l'=0}^{L} b_{n'l'}^k G_{nl,n'l'} , \tag{3.5}$$

we find that

$$\sum_{k=1}^{1/2K-1} a_k W_{nl}^k+(q/D)G_{nl,00}=(2D)^{-1}\delta_{l1}d_n . \tag{3.6}$$

Inversion of Eq. (3.6) for all n and odd l yields the unknown a_k and q.

B. Variational boundary conditions

The success of the Marshak condition, despite its arbitrariness, is not well understood.[3-5,24] For example, the retention of only odd l is not easily justified. We here introduce an alternate method based on a variational procedure for comparison.

Consider the functional

$$F=\int H(\mu)(f(0,p,\mu))^2(f^M(p))^{-1}d\vec{p}\ . \tag{3.7}$$

The unknown coefficients are determined by minimizing F. With Eq. (2.32) in Eq. (3.7), the condition $\partial F/\partial a_k=0$ leads to the following $\frac{1}{2}K-1$ equations:

$$\sum_{k'=1}^{1/2K-1} a_{k'}\sum_{n=0}^{N}\sum_{l=0}^{L} b_{nl}^{k}W_{nl}^{k'}+(q/d)W_{00}^{k} =D^{-1}\sum_{n=0}^{N} d_n W_{n1}^{k}\ . \tag{3.8a}$$

Similarly, the condition $\partial F/\partial q=0$ gives the additional equation

$$\sum_{k=1}^{1/2K-1} a_k W_{00}^{k}+q/2D=D^{-1}\sum_{n=0}^{N} d_n G_{n\,1,00}\ . \tag{3.8b}$$

Equations (3.8) are a total of $\frac{1}{2}K$ equations in $\frac{1}{2}K$ unknowns. Inversion of these equations gives the desired a_k coefficients and q.

IV. NUMERICAL RESULTS

The important quantities in this study are the spatial eigenvalues g_k that determine the rate of decay of the transient solution $f^{\rm tr}$, Eq. (2.9); the extrapolation length q that occurs in the asymptotic solution $f^{\rm as}$, Eq. (2.22), and the density profile given by the integral over the general solution $f=f^{\rm tr}+f^{\rm as}$, Eq. (2.32). These quantities depend on γ and the number of basis functions employed in the expansions of $f^{\rm tr}$ and $f^{\rm as}$. Except for the spatial eigenvalues, these also depend on the choice of boundary conditions. The main objective of the present study is to examine the convergence of these quantities as the number of basis functions is increased, their mass dependence, and the nature of $f(x,p,\mu)$.

An important aspect of the numerical work is the recognition that the collision operator in Eqs. (2.5) and (2.10) conserves particle number. Integration of Eq. (2.10) gives

$$\int p\mu R_k(p,\mu)d\vec{p}=0\ , \tag{4.1}$$

which, with Eqs. (2.11) and (2.14), implies $b_{01}^{k}=0$. This is an important point since, with Eqs. (2.23) and (2.32), we find that

$$j=2^{-1/2}\sum_k a_k e^{g_k x}b_{01}^{k}-1\ . \tag{4.2}$$

Since $b_{01}^{k}=0$, $j=-1$ is consistent with the chosen normalization. Furthermore, it can be shown that $f^{\rm tr}$ does not contribute to the K integral[2,12] defined by

$$K(x)=\int p\mu^2 U(p)f(x,p,\mu)d\vec{p}\ . \tag{4.3}$$

If $K^{\rm tr}(x)$ denotes the contribution of $f^{\rm tr}$ to $K(x)$, we have, with Eq. (2.9), that

$$K^{\rm tr}(x)=\sum_{k=1}^{\infty} a_k e^{g_k x}\int p\mu^2 U(p)R_k(p,\mu)d\vec{p}\ . \tag{4.4}$$

For a finite-order expansion, it may be shown that

$$\int p\mu^2 U(p)R_k(p,\mu)d\vec{p}=-b_{01}^{k}/\sqrt{2}g_k=0\ , \tag{4.5}$$

where Eqs. (2.11), (2.16), (2.18b), (2.29), and (2.30) have been used. Also, it may be shown that Eq. (4.5) is valid for the case $g_k=0$. It should be noted that the proof of Eq. (4.5) requires that the upper limits of the sums over n in Eqs. (2.16) and (2.29) are equal. Equation (2.32) has been written with equal upper limits of the n sums. Therefore, the distribution function calculated through the use of Eq. (2.32) will satisfy the K integral condition identically at all finite orders.

The K integral is often used in a variational calculation of q (Refs. 2 and 12) based on the fact that, as shown above, only the asymptotic solution contributes and $K(x)$ varies as $q+x$.[2] In the present method of solution, the K integral plays no direct part.

A. Spatial eigenvalues

The first step in the calculation is the evaluation of the spatial eigenvalues g_k in the transient solution. The summations in the set of equations, Eq. (2.16), are truncated at $n'=N$ and $l'=L$, which yield a set of discrete eigenvalues. It is well known that the eigenvalue spectrum has both discrete and continuous portions,[31] although the mathematical properties are not fully understood. In this paper, we are concerned with the numerical calculation of a set of discrete eigenvalues and a study of the numerical convergence as N and L are increased. In all previous work,[11,15,30] the expansion in μ has usually been restricted to no more than one or two terms. It is clear that such limited studies are insufficient to establish convergence.

The eigenvalues were calculated by diagonalizing the matrix in parentheses in Eq. (2.16), constructed

in accordance with Eqs. (2.19) and (2.20). The form of Eq. (2.16) was suitable for a numerical diagonalization procedure known as the QZ method.[32] The size of the basis set was increased and successive approximations of the eigenvalues were obtained as shown in Table I, for $\gamma=1$, and $k=1-4$. With L odd, the pairing of the eigenvalues in positive and negative pairs as discussed earlier was observed and, therefore, odd L was employed in all calculations.

Williams and Spain[31] have shown that the magnitude of the discrete eigenvalues (properly normalized) must lie in the range (0,1), while the continuous portion of the spectrum lies outside this range. The converged eigenvalues shown in Table I obviously lie in the discretum. However, most of the remaining discrete eigenvalues calculated for larger k were, in fact, in the continuum.

The magnitude of these eigenvalues is qualitatively indicative of the rate of decay of the transient solution as one recedes from the boundary. This is an important part of the study of boundary effects. The variation of the lowest-order eigenvalues versus $M=m/(m+m_1)$ is shown in Fig. 2. For mass ratios close to unity ($M\sim\frac{1}{2}$), energy exchange is efficient and the eigenvalues achieve a maximum. The boundary layer regime is consequently narrower for nearly equal mass ratios relative to the situation in the disparate mass case ($M\rightarrow 0$ or 1).

B. Extrapolation length

The calculation of the extrapolation length q depends on the choice of boundary conditions and is given by Eqs. (3.6) and (3.8) in the Marshak and variational methods, respectively. The extrapolation length was calculated with the Marshak and variational boundary conditions and for $\gamma=1$ results for several different orders are shown in Table II. Both sets of extrapolation lengths appear to be converging, but the convergence is more rapid for the Marshak conditions. The convergence for fixed N and increasing L for the Marshak boundary conditions should be noted. It is interesting to notice also the more rapid convergence of q relative to the individual eigenvalues in Table I. The converged value $q=0.937$ is in excellent agreement with the variational result 0.935 obtained by Kladnik and

TABLE I. $\gamma=1$ eigenvalues.

N \ $L=$	1	3	5	7	9	11	13
				First eigenvalue			
1	1.4154	1.0002	0.9611	0.9555	0.9547	0.954 51	0.954 48
3	1.2101	0.9042	0.8831	0.8812	0.8810	0.880 98	0.880 98
5	1.2099	0.9042	0.8831	0.8812	0.8810	0.880 971	0.880 970
7	1.2099	0.9042	0.8831	0.8812	0.8810	0.880 971	0.880 970
9	1.2099	0.9042	0.8831	0.8812	0.8810	0.880 971	0.880 970
				Second eigenvalue			
1		2.1519	1.3660	1.1995	1.1304	1.097 1	1.078 3
3	1.4199	1.0057	0.9622	0.9546	0.9532	0.952 8	0.952 8
5	1.3956	0.9855	0.9432	0.9361	0.9349	0.934 67	0.934 64
7	1.3956	0.9855	0.9432	0.9361	0.9349	0.934 64	0.934 60
9	1.3956	0.9855	0.9432	0.9361	0.9349	0.934 64	0.934 60
				Third eigenvalue			
1		2.6105	1.4165	1.2451	1.1841	1.1480	1.1221
3	2.2767	1.3226	1.1429	1.0843	1.0595	1.0473	1.0405
5	1.4860	1.0304	0.9771	0.9660	0.9634	0.9628	0.9627
7	1.4830	1.0252	0.9703	0.9586	0.9558	0.9551	0.9550
9	1.4830	1.0252	0.9703	0.9586	0.9558	0.9551	0.9550
				Fourth eigenvalue			
1			3.5183	1.7490	1.4111	1.2716	1.1995
3		2.1966	1.3423	1.1784	1.1193	1.0912	1.0749
5	1.6787	1.1373	1.0553	1.0300	1.0200	1.0155	1.0134
7	1.5345	1.0510	0.9895	0.9751	0.9713	0.9702	0.9699
9	1.5342	1.0497	0.9869	0.9716	0.9673	0.9661	0.9658

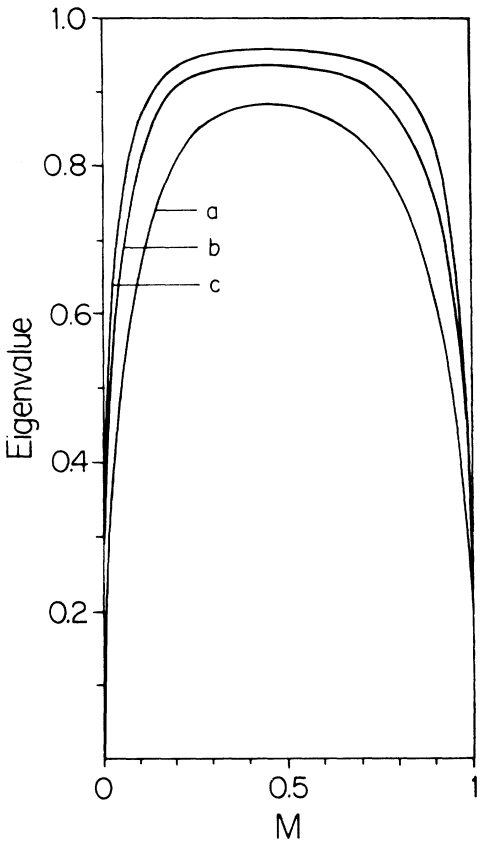

FIG. 2. Magnitude of the (a) first, (b) second, and (c) third nonzero eigenvalues; $N=9$, $L=11$.

Kuscer.[12] Conkie's result, 0.763, is too low, due to an error or to the restricted size of his basis functions in the expansion of f^{tr}, particularly in μ.

Calculations of the mass dependence of the extrapolation length were carried out with $N=9$ and $L=11$. This size of basis set was a useful compromise between accuracy and computer costs. These results are summarized in Table III and Fig. 3 for $\gamma \geq 1$ and in Table IV and Fig. 4 for $\gamma \leq 1$. From the results in Tables III and IV, it is clear that the Marshak boundary conditions are superior to the variational procedure. In particular, a useful comparison is with the one-speed case for which $q=0.7104$. As $M \to 0$, the Marshak results are approximately 0.4% below this value. Since the present method of solution of the Boltzmann equation was not designed to be especially favorable in this limit, this is considered to be good agreement. Also shown in Fig. 3 are the results obtained by Williams[13] and Arkuszewski.[14] These results were calculated by replacing the collision operator in Eq. (2.5) with an approximate separable kernel.[33] The separable kernel does not properly approximate the anisotropic scattering and the correct mass dependence for the extrapolation length is not retained. However, the analytic methods developed with the separable kernel[13,14] are useful in the solution of model problems.

For $\gamma < 1$, the extrapolation length $\tilde{q}=\sqrt{\gamma}q$ is used since q diverges as $\gamma^{-1/2}$ as $\gamma \to 0$. The results with the variational method are about 2% below the results obtained with the Marshak method. In the limit $\gamma \to 0$, $\tilde{q}$ with the Marshak method is of the order of 0.68–0.69. It might be of interest to compare this result with a calculation employing the Fokker-Planck operator which coincides with the Boltzmann collision operator in this limit.

C. Distribution function and related quantities

We chose to show the variation of the distribution function, calculated with Eq. (2.32), versus μ at

TABLE II. $\gamma=1$ extrapolation length.

N \ $L=$	1	3	5	7	9	11	13
			Variational boundary conditions				
1	0.6281	0.8311	0.8456	0.8493	0.8504	0.8507	0.8507
3	0.6432	0.8589	0.8791	0.8849	0.8868	0.8874	0.8876
5	0.6457	0.8654	0.8882	0.8956	0.8983	0.8993	0.8998
7	0.6466	0.8681	0.8923	0.9008	0.9042	0.9057	0.9063
9	0.6471	0.8695	0.8946	0.9038	0.9078	0.9096	0.9105
			Marshak boundary conditions				
1	0.8706	0.9252	0.9279	0.9281	0.9281	0.9280	0.9279
3	0.8747	0.9302	0.9336	0.9342	0.9344	0.9344	0.9344
5	0.8751	0.9310	0.9347	0.9356	0.9358	0.9359	0.9359
7	0.8753	0.9313	0.9352	0.9361	0.9365	0.9366	0.9366
9	0.8754	0.9314	0.9354	0.9364	0.9368	0.9370	0.9370

TABLE III. $\gamma \geq 1$ extrapolation lengths q for $N=9$ and $L=11$.

γ	M	Marshak	Variational
1	0.50	0.9370	0.9096
1.222	0.45	0.8933	0.8671
1.5	0.40	0.8564	0.8313
1.857	0.35	0.8250	0.8009
2.333	0.30	0.7984	0.7753
3	0.25	0.7759	0.7538
4	0.20	0.7569	0.7357
5.667	0.15	0.7410	0.7208
9	0.10	0.7278	0.7087
19	0.05	0.7170	0.6994
39	0.025	0.7123	0.6958
99	0.010	0.7097	0.6943
∞	0	Exact:	0.7104

$x=0$, that is, at the boundary. The results obtained with the Marshak boundary condition are shown in Fig. 5 for several values of p. From the results in Fig. 5, it is clear that the distribution function is peaked in the forward direction, $\mu=-1$; more so for $\gamma=1$ than for $\gamma=10$. For larger reduced speeds, the maximum of the distribution function in the forward direction is more pronounced. Of particular interest is that the boundary condition,

$$f(0,p,\mu)=0, \quad 0<\mu<1$$

is better satisfied at high p than at low p. This boundary condition was found to be less well satisfied with the variational boundary condition and is the reason for the choice of the Marshak condition in showing these results. In either case, the boundary condition cannot be satisfied exactly with the finite polynomial expansions employed in the present paper. The oscillations of f versus μ in the region $0<\mu<1$ is a consequence of this method of solution of the Boltzmann equation.

An important aspect of the present work is to show the extent of the departure from hydrodynamic behavior near the boundary at $x=0$. This can be shown in a variety of ways and we have chosen to display results for the density

$$n(x)=\int f(x,p,\mu)d\vec{p} = \sum_{k=1}^{1/2K-1} a_k e^{g_k x} b_{00}^k + D^{-1}(q+x) \tag{4.6}$$

in Fig. 6 and for $|D\,dn(x)/dx|$ in Fig. 7. For large x, $n(x)$ approaches $n^{as}(x)$ given by Eq. (2.25) and $|D\,dn(x)/dx|$ approaches unity. The extent of the departure from hydrodynamic behavior depends on the extrapolation length q, the eigenvalues g_k, and the coefficients a_k. Each of these quantities exhibits a different mass dependence that has not been examined in detail. Figures 6 and 7 show the

TABLE IV. $\gamma \leq 1$ extrapolation lengths $\tilde{q}$ for $N=9$ and $L=11$.

γ	M	Marshak	Variational
1	0.50	0.9370	0.9096
0.8181	0.55	0.8944	0.8685
0.6667	0.60	0.8581	0.8336
0.5385	0.65	0.8267	0.8036
0.4286	0.70	0.7992	0.7776
0.3333	0.75	0.7749	0.7547
0.2500	0.80	0.7533	0.7346
0.1765	0.85	0.7338	0.7168
0.1111	0.90	0.7161	0.7009
0.0526	0.95	0.7000	0.6870
0.0101	0.99	0.6881	0.6770
0.0010	0.999	0.6856	0.6749

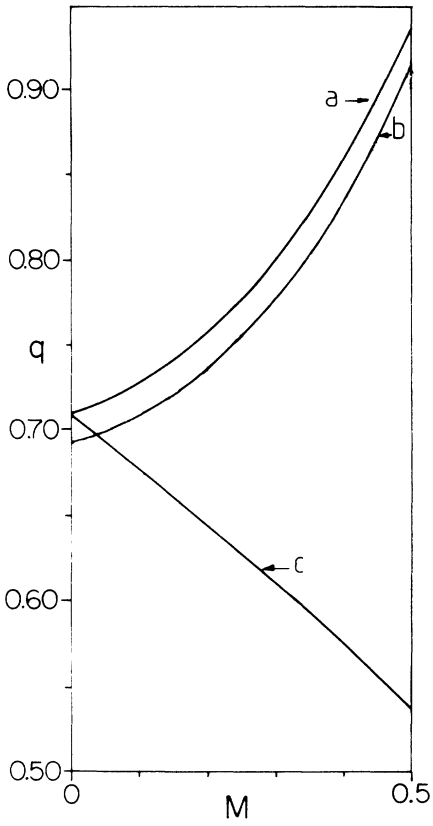

FIG. 3. Extrapolation length q vs M for $N=9$, $L=11$. (a) Marshak, (b) variational, (c) synthetic kernel (Ref. 13).

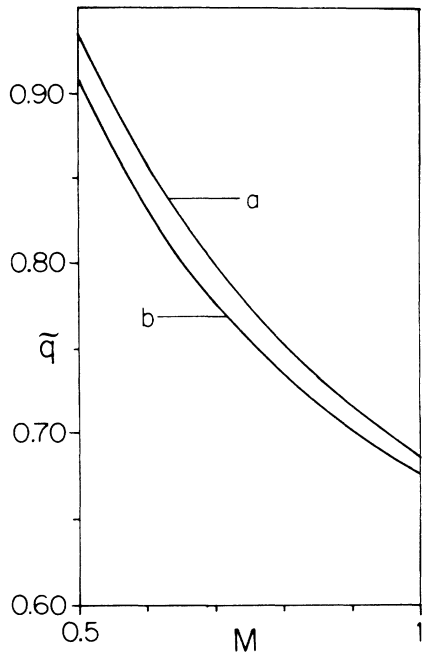

FIG. 4. Extrapolation length $\tilde{q}$ vs M for $N=9$, $L=11$. (a) Marshak, (b) variational.

approach to hydrodynamic behavior in a distance of the order of several mean-free paths. This region of nonhydrodynamic behavior is of greater extent for smaller γ, although there does not appear to be a strong mass dependence for the range of values of γ studied.

Since there is a preferential loss of energetic particles from the medium, the temperature $T(x)$ of test particles is somewhat less than the temperature T_1 of the medium. A local temperature may be defined as

$$\tfrac{3}{2}\bar{n}(r)kT(r)=\int \tfrac{1}{2}m(\vec{v}-\vec{V})^2\bar{f}(r,\vec{v})d\vec{v}\ , \tag{4.7}$$

where $\vec{V}=\vec{\bar{j}}/\bar{n}(r)$ is the flow velocity

$$\vec{\bar{j}}=\int \vec{v}\bar{f}(r,\vec{v})\vec{d}\vec{v}$$

and

$$\bar{n}(r)=\int \bar{f}(r,\vec{v})d\vec{v}\ .$$

Substitution of Eq. (2.32) yields

$$T(x)/T_1=[2/3n(x)]\sum_k a_k e^{g_k x}\{(\tfrac{3}{2})^{1/2}b_{10}^k+[\tfrac{3}{2}+n(x)^{-2}]b_{00}^k\}$$
$$+[2/3n(x)D]\{(q+x)[\tfrac{3}{2}+n(x)^{-2}]-2D/n(x)\}\ . \tag{4.8}$$

The ratio $T(x)/T_1$ is shown in Fig. 8 and the cooling of test particles as the boundary is approached is observed. The ratio $T(x)/T_1$ decreases with increasing γ due to the reduced efficiency of energy transfer as γ departs from unity.

V. SUMMARY

A numerical solution of the Milne problem has been presented without approximation to the Boltzmann collision operator. The method uses an

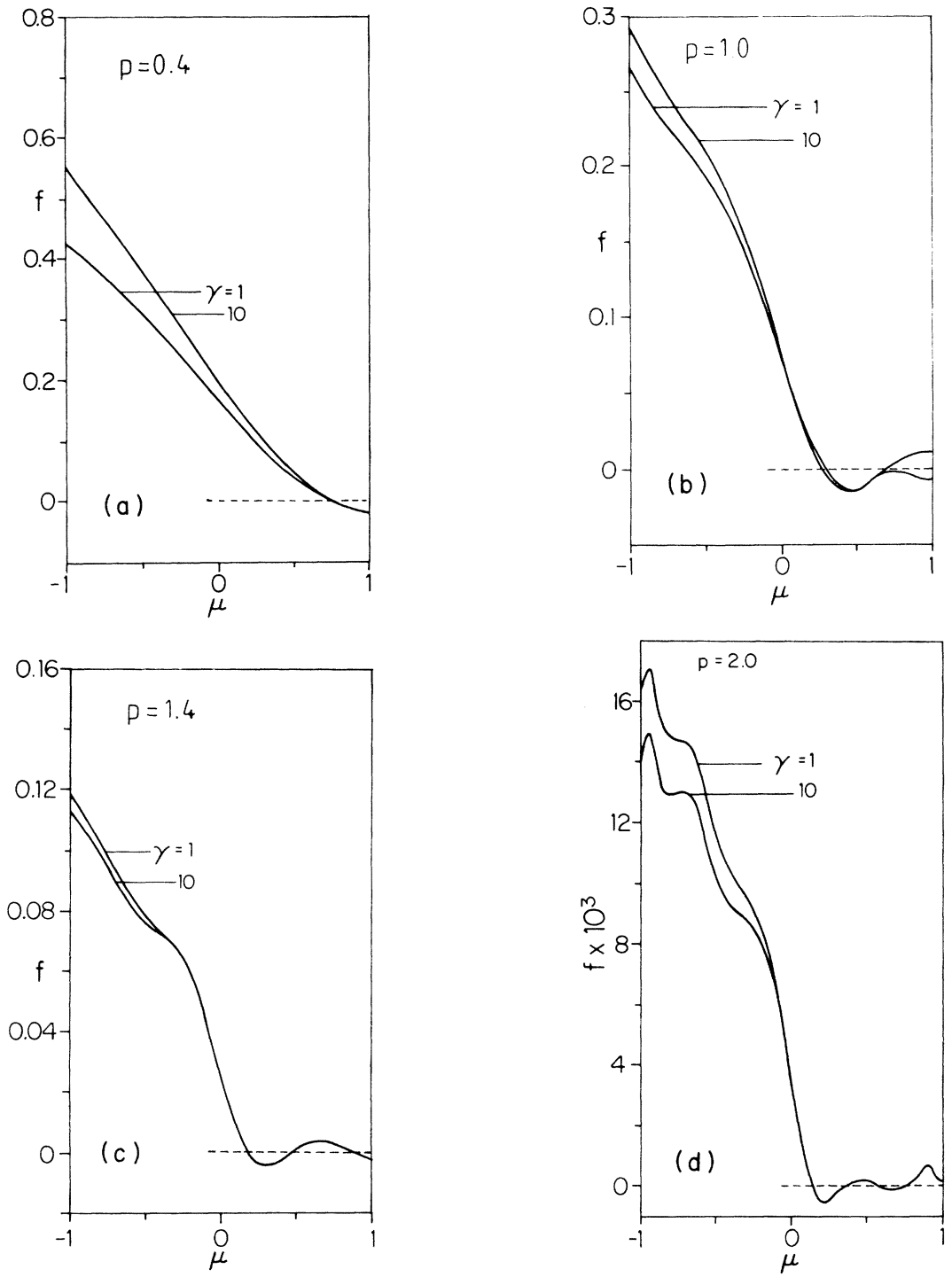

FIG. 5. Surface distribution function $f(x=0,p,\mu)$ vs μ at $N=9$, $L=11$ with Marshak boundary conditions for (a) $p=0.4$, (b) $p=1.0$, (c) $p=1.4$, (d) $p=2.0$.

expansion of the distribution function in Burnett polynomials. The calculation naturally splits into three parts. First, the eigenvalues and eigenfunctions of the transient part of the distribution function are determined by the generalized eigenvalue Eq. (2.16). Second, the asymptotic solution expansion coefficients d_n and the diffusion coefficient are given by Eqs. (2.30) and (2.31). Finally, the eigen-

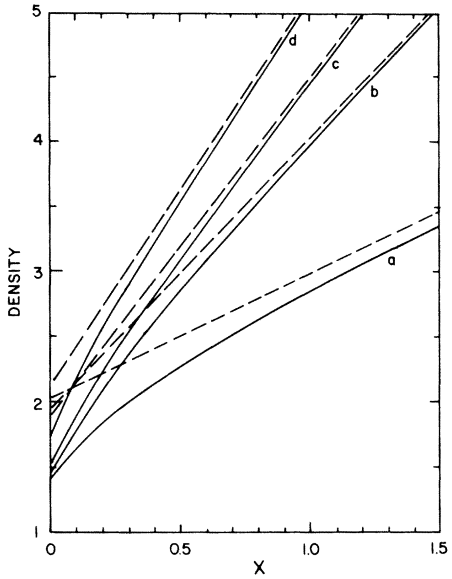

FIG. 6. Number density for $N=9$, $L=11$ with Marshak boundary conditions for (a) $\gamma=\frac{1}{9}$, (b) $\gamma=1$, (c) $\gamma=10$, (d) $\gamma=\infty$ or one-speed results of Table III in LeCaine (Ref. 34); — — — $n^{as}(x)$.

function expansion coefficients a_k and the extrapolation length q are given by Eqs. (3.1), (3.7), and (3.9) in the Mark, Marshak, and variational methods, respectively. The general solution, Eq. (2.32), at any finite order, satisfies exactly conservation of mass and the K integral.

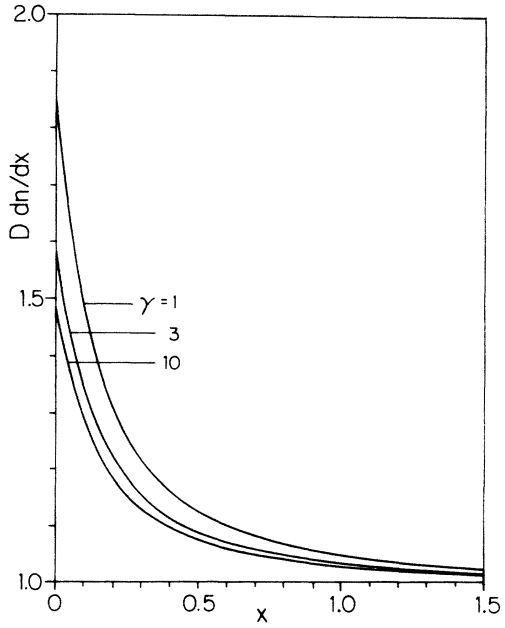

FIG. 7. $|D\,dn/dx|$ at $N=9$, $L=11$ with Marshak boundary conditions.

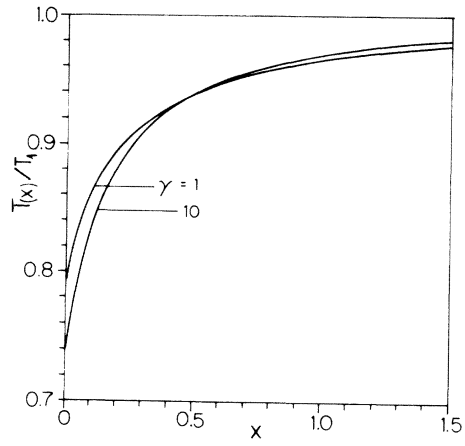

FIG. 8. Ratio of test particle kinetic temperature to medium temperature at $N=9$, $L=11$ with Marshak boundary conditions.

Convergence in the above quantities has been verified by increasing the size of the basis sets. Our numerical results show the importance of verifying convergence of the expansion in *both* variables. The rate of convergence has been used in choosing among different methods for boundary conditions. As the Marshak method gave the best convergence, it was adopted as the preferred method. Calculations of associated quantities, such as density, $D\,dn/dx$, kinetic temperature, and angular and speed distributions, exhibited reasonable behavior.

Our result for the extrapolation length at $\gamma=1$, $q=0.937$, is in good agreement with $q=0.935$ obtained by Kladnik and Kuscer[12] in a variational calculation. This agreement suggests that variational methods[12,18,19] yield accurate results for extrapolation lengths and slip coefficients, although results for other quantities may not be as accurate. It would be of interest to extend Kladnik and Kuscer's calculation to mass ratios $\gamma\neq 1$.

In Fig. 3, a comparison of the extrapolation length as a function of mass ratio for the hard-sphere Boltzmann and separable collision kernels has been given. A possible explanation for the different behavior can be given if one assumes that $n^{as}(x=0)$ is approximately independent of γ and the detailed mass-ratio dependence of the diffusion coefficient is taken into account. As γ decreases from infinity the hard-sphere Boltzmann diffusion coefficient increases, implying a decreasing $dn^{as}(x)/dx$ (for fixed flux). This flatter density profile must be extrapolated further back along the negative x axis to reach $n^{as}=0$. Therefore, this argument predicts that the hard-sphere extrapolation length should increase for decreasing γ, as is ob-

served. On the other hand, the separable kernel diffusion coefficient decreases with decreasing γ and, hence, the separable kernel extrapolation length should decrease with decreasing γ, as is also observed. The separable kernel is a useful analytic device but is not a realistic model of the collision operator for all mass ratios γ.

ACKNOWLEDGMENTS

This research was supported by a grant from the Natural Sciences and Engineering Research Council of Canada. One of us (B. S.) is grateful for the hospitality extended to the author at Le Service d'Aeronomie, Verrieres-le-Buisson, France, where a portion of this work was done. Financial assistance from the Cooperative Research Programme between the National Research Council of Canada and the Conseil Nationale de Recherches Scientifique of France is gratefully acknowledged. The other author (M. J. L.) wishes to express his gratitude to Dr. Denny R. S. Ko for the assistance of Dynamics Technology, Inc. in the preparation of the manuscript.

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