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The structure of the stationary kinetic boundary layer for the linear BGK equation

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Abstract. Recently, very accurate numerical methods for solving kinetic boundary layer problems for linear kinetic equations have been developed. To test such methods, detailed information about exactly solvable models can be very helpful. To this purpose we present results for the stationary, 1D linear BGK equation, obtained by the singular eigenfunction method, that extend results already known in the literature, both in scope and in precision. Special attention is paid to the nature of the singularity in the distribution function for small velocities near the boundary; this singularity cannot be reproduced exactly by the numerical methods available. Explicit expressions are presented for the Milne problem and for the albedo problem with input particles of a single velocity. We compare the results with those of a recently developed variant of the two-stream moment method. We find excellent agreement, except close to the singularity; for many quantities of interest, the accuracy obtainable by the novel two-stream moment method cannot be reproduced with comparable numerical effort by evaluation of the exact solution.

1. Introduction and survey

The BGK equation, proposed by Bhatnagar *et al* [1], and independently by Welander [2], is the simplest kinetic equation; the Boltzmann collision operator is replaced by a simple relaxation towards local equilibrium. Its linear version can be solved exactly for a number of cases in which the solution depends on a single space coordinate [3, 4], i.e. the solution can be obtained by quadratures or by the solution of (singular) integral equations in one variable. In particular, the linear BGK equation furnished the earliest and simplest examples of exactly solvable kinetic boundary layer problems [3, 4].

The availability of exact solutions means that the BGK equation may be used as a test case for approximate and numerical schemes for solving kinetic boundary layer problems. As such it was used in some recent papers [5, 6] on methods for solving planar problems with several boundary conditions by variants of the moment method. In one of these papers [6] we developed a highly accurate two-stream moment method and compared its results with exact information, both for the BGK and for the Klein-Kramers [7-9] equation. Since much of the required information about the BGK equation was not available in the literature in an immediately usable form, the comparison needed in [6] required an extension of the known results on the BGK equation. Many such results were quoted without proof in [6]; in the present paper they will be presented in a systematic way, and their derivation will be outlined.

Our results in this paper extend known results mainly in two directions. First, we provide a systematic study of the analytic structure of the singularity of the stationary half-space solutions at the confining wall at zero velocity. Since such a singularity cannot be reproduced exactly by the moment methods, which approximate the solution by a sequence of piecewise analytic functions, the behaviour near the singularity provides the most sensitive test for these approximation schemes. Second, we present some techniques that allow us to replace the singular integral equations that appear in some kinetic boundary layer problems by non-singular ones that are more amenable to numerical solution. Though our methods can also be applied to the Laplace transform of the time-dependent linear BGK equation, and to slab geometries, we shall confine ourselves in this paper to stationary problems in half-space geometries, but for a few remarks in the concluding section.

In section 2 we give the explict form of the simple stationary linear BGK equation treated in this paper. In addition we present the singular eigenfunctions [10, 11] and their half-range completeness and orthogonality properties, which enable us to reduce the simplest boundary layer problems to quadratures. We also give some auxiliary formulae needed later in the paper. In section 3 we discuss the simplest boundary layer problems, in which the wall absorbs (or transmits) all particles impinging upon it. When the particle source is at infinity we thus obtain the Milne problem; for a source situated at the wall we obtain the albedo problem. We discuss in particular the singularity in those solutions at the wall. In addition to the albedo problems discussed in [6] we discuss the case of a source that emits particles with a single velocity. The solution thus obtained is (up to a constant) equal to the Green function for the BGK equation with absorbing wall for the special case that the source point lies at the wall. The results are compared with those of the two-stream moment method presented in [6].

In section 4 we discuss the case that the wall reflects some of the particles, elastically or inelastically. In this case, the singular eigenfunction method reduces the problem to a solution of a singular integral equation. We reduce this equation to a regular one and discuss a solution method that is sufficiently accurate to allow a comparison with the moment method presented in [6], though it was not possible to obtain an accuracy comparable to that of the two-stream moment method without excessive numerical effort. In the concluding section we discuss some possible extensions of our methods to slightly more complicated problems. Some auxiliary formulae, especially for the asymptotic evaluation of integrals needed to determine the nature of the singularity discussed in section 3, are discussed in an appendix.

2. The BGK equation and its singular eigenfunctions

The stationary linear BGK equation for the distribution function $f(u, x)$ of velocity u and position x of an assembly of (monoatomic) gas molecules reads [4]

$$u\frac{\partial}{\partial x}f(u,x) = -f(u,x) + \phi_0(u)\int_{-\infty}^{+\infty} du'\, f(u',x) \tag{2.1}$$

where $\phi_0(u)$ is the normalized 1D Maxwell distribution

$$\phi_0(u) = (2\pi)^{-1/2}\exp[-u^2/2]. \tag{2.2}$$

It is obtained by replacing the Boltzmann collision operator by a simple relaxation towards total equilibrium. In (2.1) velocities are measured in units of the mean thermal velocity and lengths in terms of the mean free path. This equation has special solutions of the form

$$f(u,x)=\mathrm{e}^{-x/\lambda}g_\lambda(u)\phi_0(u). \tag{2.3}$$

By substituting (2.3) into (2.1) and integrating over u one immediately sees that solutions of type (2.3) carry no current. As noted by van Kampen [10] and Case [11], the generalized eigenfunctions g_λ have the form

$$g_\lambda(u)=P\frac{\lambda}{\lambda-u}+p(\lambda)\delta(\lambda-u) \tag{2.4}$$

where $p(\lambda)$ follows from the normalization requirement

$$P\int_{-\infty}^{+\infty}\mathrm{d}u\,\phi_0(u)g_\lambda(u)=1 \tag{2.5}$$

with P denoting the principal value, and is given by

$$p(\lambda)\phi_0(\lambda)=1-\lambda\sqrt{2}\,F_\mathrm{D}(\lambda/\sqrt{2}) \tag{2.6}$$

where $F_\mathrm{D}(v)$ denotes Dawson's integral

$$F_\mathrm{D}(v)=\exp[-v^2]\int_0^v\mathrm{d}t\,\exp[t^2]. \tag{2.7}$$

In addition to the generalized eigenfunctions $g_\lambda(u)$ belonging to the continuous spectrum, one has the normalizable eigenfunction $\phi_0(u)$, belonging to $\lambda=\infty$, and the associated function

$$\phi_1(u,x)=(x-u)\phi_0(u). \tag{2.8}$$

The set of functions

$$\{\phi_0(u);\ u\phi_0(u);\ g_\lambda(u)\phi_0(u)\ \text{with}\ -\infty<\lambda<\infty\} \tag{2.9}$$

is orthogonal and complete on the real line $-\infty<u<\infty$ [4]. For boundary layer problems, more useful properties are the so-called half-range orthogonality and completeness properties: in terms of the scalar product†

$$(f,g)_+=P\int_0^\infty\mathrm{d}u\,w(u)f(u)g(u) \tag{2.10a}$$

$$w(u)=u\phi_0(u)Q(u)\qquad Q(u)=\exp\left\{\int_0^\infty\mathrm{d}t\frac{t\ln(t+u)}{C(t)}\right\} \tag{2.10b}$$

$$C(u)=u\phi_0(u)[\pi^2u^2+p(u)^2] \tag{2.10c}$$

the half-range orthogonality can be expressed as [4, 12, 13]

$$(1,1)_+=1\qquad (1,g_\lambda)_+=0$$
$$(g_\lambda,g_\mu)_+=C(\lambda)Q(\lambda)\delta(\lambda-\mu)\qquad \text{for}\ \lambda,\mu>0 \tag{2.11}$$

and the half-range completeness relation reads

$$1+P\int_0^\infty\mathrm{d}\lambda\frac{g_\lambda(u)g_\lambda(v)}{C(\lambda)Q(\lambda)}=\frac{\delta(u-v)}{w(u)}. \tag{2.12}$$

† The expression (2.10b) for $Q(u)$ follows from that given by Cercignani [4] by partial integration of the $\tan^{-1}$ function.

The relations (3.10) and (3.12) imply that the set of functions

$$\{\phi_0(u);\ g_\lambda(u)\phi_0(u), \text{ with } 0<\lambda<\infty\} \tag{2.13}$$

is orthogonal and complete on the half-line $0<u<\infty$ with respect to (2.10*a*). In particular, any function $g(u)$ with

$$\int_0^\infty \mathrm{d}u\, u^2 g(u)<\infty \tag{2.14}$$

can be written uniquely in the form

$$g(u)=\phi_0(u)\left[A_0+P\int_0^\infty \mathrm{d}\lambda\, A(\lambda)g_\lambda(u)\right] \qquad u>0 \tag{2.15a}$$

$$A_0=(g,\phi_0^{-1})_+ \qquad A(\lambda)=\frac{1}{C(\lambda)Q(\lambda)}(g,\phi_0^{-1}g_\lambda)_+. \tag{2.15b}$$

The representation (2.15) can be derived from (2.11) and (2.12). A useful identity for albedo problems is

$$\frac{1}{u}=1+P\int_0^\infty \frac{\mathrm{d}\lambda\, g_\lambda(u)}{C(\lambda)Q(\lambda)} \tag{2.16}$$

which is derived from (2.12) by multiplying with $w(v)\ v^{-1}$ and integrating over $v>0$. In evaluating the integrals we used the identities

$$([t+u]^{-1},1)_+=Q(t)^{-1} \qquad \text{with } Q(0)=1 \tag{2.17a}$$

which follows from (3.35) of [4], and

$$([t-u]^{-1},1)_+=-p(t)w(t)t^{-1} \tag{2.17b}$$

which follows from (2.17*a*) and $(1,g_\lambda)_+=0$ (see (2.11)). The identity

$$(u^{-1},g_\lambda)_+=1 \tag{2.18}$$

follows straightforwardly from (2.17*a*) and (2.17*b*), whereas $(1,g_\lambda)_+=0$ and $(1,1)_+=1$ lead to

$$(u,g_\lambda)_+=-\lambda. \tag{2.19a}$$

The corresponding expression for the discrete eigenfunction

$$(u,1)_+=\int_0^\infty \mathrm{d}u\, uw(u)=\int_0^\infty \frac{\mathrm{d}t\, t^2}{C(t)}\equiv x_{\mathrm{M}}^{\mathrm{BGK}} \tag{2.19b}$$

is a variant of (4.8) of [4]. The quantity $x_{\mathrm{M}}^{\mathrm{BGK}}$ is the Milne length for the BGK equation, as will be shown in the next section. The identities (2.17)-(2.19) will be needed in the subsequent sections. Singular integrals such as that occurring in (2.15*b*) can be reduced to regular ones by means of

$$P\int_0^\infty \mathrm{d}x \frac{x\phi_0(x)}{x-z}h(x)=\int_0^\infty \mathrm{d}x\, x\phi_0(x)\frac{h(x)-h(z)}{x-z}+h(z)P\int_0^\infty \mathrm{d}x\frac{x\phi_0(x)}{x-z} \tag{2.20a}$$

and

$$P\int_0^\infty \mathrm{d}x\frac{x\phi_0(x)}{x-z}=p(z)\phi_0(z)-\int_0^\infty \mathrm{d}x\frac{x\phi_0(x)}{x+z} \tag{2.20b}$$

where the latter identity follows from (2.5), (2.4) and the normalization condition for $\phi_0(z)$.

For future use we also note that the behaviour of the function $p(\lambda)$ defined in (2.6) for small and large λ follows from

$$p(\lambda)\phi_0(\lambda) \approx -\lambda^{-2} \qquad \text{for } \lambda \to \infty \tag{2.21a}$$

$$p(\lambda) = \sqrt{2\pi}\left[1 - \sum_{n=0}^{\infty} \frac{(2n-1)!!}{(2n+2)!}\lambda^{2n+2}\right]. \tag{2.21b}$$

For the function $\lambda/C(\lambda)$, with $C(\lambda)$ defined in (2.10*c*), this implies

$$\lambda/C(\lambda) \approx \lambda^4\phi_0(\lambda) \qquad \text{for } \lambda \to \infty \tag{2.22a}$$

$$\lambda/C(\lambda) = \frac{1}{\sqrt{2\pi}}[1 - \tfrac{1}{2}\lambda^2(\pi - 3)] + \mathcal{O}(\lambda^4) \qquad \text{for small } \lambda. \tag{2.22b}$$

Finally, for $Q(\lambda)$ we find, using the techniques described in the appendix,

$$Q(\lambda) = 1 - \frac{\lambda \ln \lambda}{\sqrt{2\pi}} + 0.724\,71\ldots\lambda + \frac{1}{4\pi}\lambda^2(\ln\lambda)^2 - \frac{0.724\,71\ldots}{\sqrt{2\pi}}\lambda^2\ln\lambda + \mathcal{O}(\lambda^2) \tag{2.23a}$$

whereas in the limit of large λ an expansion of the logarithm in the integrand leads to

$$Q(\lambda) \approx \lambda + x_{\mathrm{M}}^{\mathrm{BGK}} + \mathcal{O}(\lambda^{-1}) \tag{2.23b}$$

where we used the results

$$\int_0^\infty \mathrm{d}t \frac{t}{C(t)} = 1 \qquad \int_0^\infty \mathrm{d}t \frac{t^2}{C(t)} \equiv x_{\mathrm{M}}^{\mathrm{BGK}} = 1.437\,111\,685\,7600\ldots. \tag{2.24}$$

3. The Milne and albedo problems

The most general solution of (2.1) that increases no faster than linearly with x is given by

$$f(u,x) = \phi_0(u)\left[A_0 + A_1(x-u) + P\int_0^\infty \mathrm{d}\lambda\, A(\lambda)g_\lambda(u)\,\mathrm{e}^{-x/\lambda}\right]. \tag{3.1}$$

The associated density in position space is

$$n(x) = \int_{-\infty}^{+\infty} \mathrm{d}u\, f(u,x) = A_0 + A_1 x + \int_0^\infty \mathrm{d}\lambda\, A(\lambda)\,\mathrm{e}^{-x/\lambda} \tag{3.2}$$

as follows from the normalization condition (2.5); the particle current equals

$$j(x) = \int_{-\infty}^{+\infty} \mathrm{d}u\, u f(u,x) = -A_1. \tag{3.3}$$

(As noted after (2.3), the terms containing A_0 and $A(\lambda)$ carry no current.) The albedo solution $f_g(u,x)$ for the input distribution $g(u)$ is characterized by

$$A_1^g = 0 \qquad f_g(u,0) = g(u) \text{ for } u > 0 \tag{3.4}$$

and it follows from the half-range completeness that A_0^g and $A^g(\lambda)$ are given by (2.15*b*). Physically, this corresponds to the situation that particles are injected into the half-space at the wall $x=0$ with velocity distribution $g(u)$ and absorbed (or transmitted) upon return to the wall. The Milne solution $f_M(u,x)$ is characterized by

$$A_1^M=1 \qquad f_M(u,0)=0 \text{ for } u>0. \tag{3.5}$$

Since $f_M(u,x)-(x-u)\phi_0(u)$ is the albedo solution for $g(u)=u\phi_0(u)$, the coefficients in the Milne solution are found by comparing (2.19) and (2.15b), and are given by

$$A_0^M=x_M^{BGK} \qquad A^M(\lambda)=-\lambda[C(\lambda)Q(\lambda)]^{-1}. \tag{3.6}$$

Both the Milne and the albedo solution exhibit a jump at $u=0$ for $x=0$, but not for $x>0$. To show this we consider

$$\begin{aligned} S(x) &\equiv \lim_{u\downarrow 0}[f(-u,x)-f(u,x)] \\ &=\lim_{u\downarrow 0}\frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}\lambda[g_\lambda(-u)-g_\lambda(u)]A(\lambda)\,\mathrm{e}^{-x/\lambda}. \end{aligned} \tag{3.7a}$$

Since the first term in (2.4) is continuous at $u=0$, only the δ-function part contributes and we obtain

$$S(x)=\lim_{u\downarrow 0}\left(\frac{-1}{\sqrt{2\pi}}\right)p(u)A(u)\,\mathrm{e}^{-x/u}=-A(0)\lim_{u\downarrow 0}\mathrm{e}^{-x/u} \tag{3.7b}$$

where we have used (2.21b). We thus obtain

$$S(0)=-A(0) \qquad S(x)=0 \text{ for } x>0. \tag{3.8}$$

For $x>0$ the value $f(0,x)$ is given by

$$f(0,x)=\frac{1}{\sqrt{2\pi}}n(x) \tag{3.9}$$

as follows from a comparison of (3.1) and (3.2); for $x\downarrow 0$ this approaches the limiting value of $f(u,0)$ for negative u. The appearance of $A(0)$ in (3.8) is not too surprising: the nature of the singularity is determined by those components in (3.1) that decay most rapidly in space, as we also saw for the case of the Klein–Kramers equation [9].

In the remainder of this section we shall first discuss the Milne solution somewhat more fully and then add a few remarks on some albedo solutions. The condition that $f^M(u,0)$ should vanish for $u>0$ reads

$$\phi_0(u)\left[A_0^M-u+P\int_0^\infty \mathrm{d}\lambda\frac{\lambda A^M(\lambda)}{\lambda-u}+p(u)A^M(u)\right]=0 \qquad \text{for } u>0. \tag{3.10}$$

In the limit $u\downarrow 0$ the last term in square brackets approaches -1, as is clear from (3.6) and (2.21)-(2.23); the limiting value of the principal value integral will be discussed more fully in the appendix. The result obtained is

$$A_0^M+\int_0^\infty \mathrm{d}\lambda\, A^M(\lambda)=n^M(0)=1 \tag{3.11}$$

where we used (3.2). To obtain an impression of the nature of the singularity of f_M near $u=x=0$ we consider the approach towards the singularity along the lines $x=\alpha u$, $u>0$. There we have

$$f(u,\alpha u)=\phi_0(u)\left[A_0^M+u(\alpha-1)+P\int_0^\infty \mathrm{d}\lambda\frac{\lambda A^M(\lambda)}{\lambda-u}\mathrm{e}^{-\alpha u/\lambda}+A^M(u)p(u)\,\mathrm{e}^{-\alpha}\right]$$
$$\text{for } u>0,\ \alpha>0. \tag{3.12}$$

For $u\downarrow 0$ this aproaches

$$\lim_{u\downarrow 0} f(u, \alpha u) = \frac{1}{\sqrt{2\pi}}\left\{A_0^{\mathrm{M}} + \int_0^\infty \mathrm{d}\lambda\, A^{\mathrm{M}}(\lambda) - \mathrm{e}^{-\alpha}\right\} = \frac{1}{\sqrt{2\pi}}(1 - \mathrm{e}^{-\alpha}) \qquad (\alpha > 0) \quad (3.13a)$$

where we used (3.11) and treated the principal value integral using the techniques described in the appendix. For $\alpha < 0$ the last term in square brackets in (3.12) is missing and we obtain

$$\lim_{u\downarrow 0} f(-u, \alpha u) = \frac{1}{\sqrt{2\pi}} \qquad \alpha > 0. \qquad (3.13b)$$

The behaviour of $f(u, x)$ near the singularity is shown in figure 1, together with the result of the two-stream method [6], in which the precise nature of the singularity can, of course, not be reproduced faithfully. For albedo solutions, a singularity similar to that in (3.13) appears:

$$\lim_{u\downarrow 0} f_g(u, \alpha u) = \frac{n^g(0)}{\sqrt{2\pi}} + A^g(0)\,\mathrm{e}^{-\alpha} \qquad \text{for } u > 0 \qquad (3.14a)$$

$$\lim_{u\downarrow 0} f_g(-u, \alpha u) = \frac{n^g(0)}{\sqrt{2\pi}} \qquad \text{for } u > 0. \qquad (3.14b)$$

To discuss the behaviour of the Milne solution near the singularity we use the identity

$$u + A_0^{\mathrm{M}} + \int_0^\infty \mathrm{d}\lambda \frac{\lambda}{\lambda + u} A^{\mathrm{M}}(\lambda) = Q(u) \qquad (3.15)$$

which follows from (3.36) of [4] using (3.6) and (2.17a); a simple corollary is

$$f_{\mathrm{M}}(-u, 0) = \phi_0(u) Q(u). \qquad (3.16)$$

Hence the small-u expansion for $f_{\mathrm{M}}(-u, 0)$ follows immediately from (2.23a). For the density $n^{\mathrm{M}}(x)$ the asymptotic analysis of the integral (3.2) with the special values (3.6) yields

$$n^{\mathrm{M}}(x) = 1 - \frac{1}{\sqrt{2\pi}} x \ln x + \alpha x + \mathcal{O}(x^2 \ln^2 x) \qquad (3.17a)$$

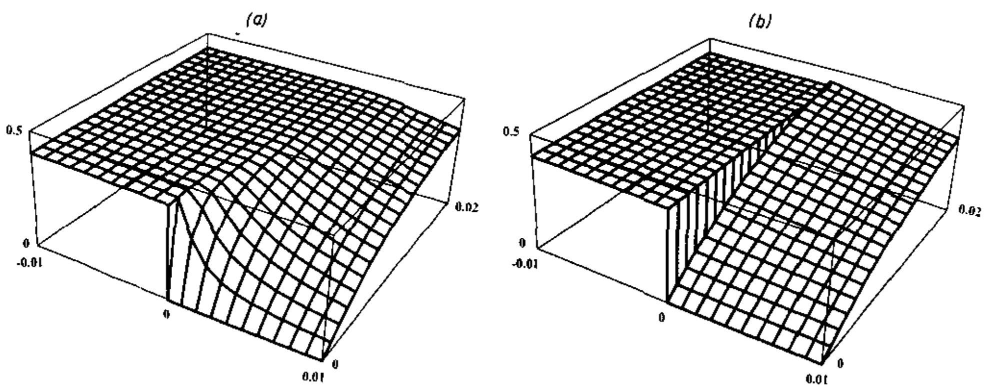

Figure 1. (a) The Milne solution $f^{\mathrm{M}}(u, x)$ in the immediate vicinity of the singularity at $u = x = 0$, for $-0.01 \leqslant u \leqslant 0.01$ and $0 \leqslant x \leqslant 0.02$ as calculated from the exact solution. (b) The same quantity as in (a), as calculated from the $N = 28$ two-stream moment method.

with

$$\alpha = 1 + \lim_{x \downarrow 0} \left\{ \frac{1}{\sqrt{2\pi}} \ln x + \frac{1}{x} \int_0^\infty d\lambda\, A^M(\lambda)[e^{-x/\lambda} - 1] \right\} \approx 0.893\,3826. \tag{3.17b}$$

The values for $n^M(x)$ for several x obtained from the exact expression and from the $N = 28$ two-stream approximation are given in table 1. We see that, as expected, the logarithmic singularity for small x in (3.17a) is not reproduced very well; however, the errors in $n^M(x)$ never exceed 10^{-3}, and they have gone down to a few parts in 10^{-7} for $x = 1$.

For the albedo problem, some special results for input distributions of the type

$$g_{\alpha,\beta}(u) \approx u^\alpha \exp[-\beta u^2/2] \tag{3.18}$$

were given in [6]. In the present paper we present some results on the monoenergetic input

$$g(u) = u_0^{-1} \delta(u - u_0). \tag{3.19}$$

From (2.15) we immediately see

$$A_0 = n(\infty) = Q(u_0) \qquad A(\lambda) = \frac{Q(u_0) g_\lambda(u_0)}{C(\lambda) Q(\lambda)} \qquad \text{for } \lambda \neq u_0. \tag{3.20}$$

The treatment of the singularity at $\lambda = u_0$ follows from the completeness relation (2.12), from which we deduce

$$f(u, x) = \phi_0(u) Q(u_0) \left[1 + P \int_0^\infty d\lambda \frac{g_\lambda(u) g_\lambda(u_0)\, e^{-x/\lambda}}{C(\lambda) Q(\lambda)} \right]. \tag{3.21}$$

In particular we obtain, using (2.16) and (2.5),

$$n(0) = \int_{-\infty}^{+\infty} du\, f(u, 0) = Q(u_0) u_0^{-1}. \tag{3.22}$$

To evaluate (3.21) we first write, using (2.4),

$$g_\lambda(u) g_\lambda(u_0) = P \frac{\lambda^2}{(\lambda - u)(\lambda - u_0)} + P \frac{\lambda p(\lambda)}{\lambda - u} \delta(\lambda - u_0)$$

$$+ P \frac{\lambda p(\lambda)}{\lambda - u_0} \delta(\lambda - u) + p^2(\lambda) \delta(\lambda - u) \delta(\lambda - u_0). \tag{3.23}$$

Table 1. The Milne density profile $n^M(x)$ for several values of x as calculated from the exact expression (ex), from the $N = 28$ two-stream moment method ($2N$), and from the part (3.17a) of the asymptotic small x expansion (as). The last column gives the error Δ_{2N} of the ($2N$) results relative to the exact ones.

x	$n^M(x)$ (ex)	$n^M(x)$ ($2N$)	$n^M(x)$ (as)	Δ_{2N}
0	1	$1 + 3 \times 10^{-14}$	1	3×10^{-14}
10^{-3}	1.003 652 913	1.003 041 578	1.003 6492	-6.09×10^{-4}
10^{-2}	1.027 524 97	1.027 3328	1.027 3058	-1.87×10^{-4}
10^{-1}	1.191 991 339	1.191 875 49	1.181 1981	-9.71×10^{-5}
0.2	1.340 348 47	1.340 375 06	1.307 0911	1.98×10^{-5}
0.5	1.726 107 69	1.726 102 21	1.584 9541	-3.17×10^{-6}
1.0	2.300 090 59	2.300 091 046	1.893 3826	1.98×10^{-7}

For $u \neq u_0$ we therefore have

$$g_\lambda(u)g_\lambda(u_0) = \frac{\lambda}{u-u_0}[g_\lambda(u) - g_\lambda(u_0)] \qquad (u \neq u_0). \tag{3.24}$$

If we substitute this result into (3.21) and compare with the results (3.1) and (3.6) for the Milne solution f_M we obtain

$$f(u,x) = \frac{-\phi_0(u)Q(u_0)}{u-u_0}\left[\frac{f_M(u,x)}{\phi_0(u)} - \frac{f_M(u_0,x)}{\phi_0(u_0)}\right] + \frac{\delta(u-u_0)}{u_0}\,\mathrm{e}^{-x/u_0}. \tag{3.25}$$

The coefficient of the δ-function in (3.25) can be obtained from the 'physical' argument that the particles injected into the system at $x=0$ with velocity u_0 are scattered with unit rate as they move into the half-space $x>0$. A formal derivation is given in the appendix.

The expression (3.25) is the Green function for the BGK equation with absorbing boundary at $x=0$ for the special case of a source point located at $x=0$. It can therefore be used to express the albedo solution for an arbitrary input function in terms of the Milne solution. The function (3.25) is plotted in figure 2 for $x=0$ and $x=1$, together with the two-stream moment result, for $u_0=2$. For $u<0$ the results obtained with the two methods agree to within the accuracy of figure 2; for $u>0$ the moment method of course yields a rather poor approximation to the δ-function. Some numerical results are given in table 2. We see that the two-stream method gives highly accurate results for moments, except for very high or very low u_0.

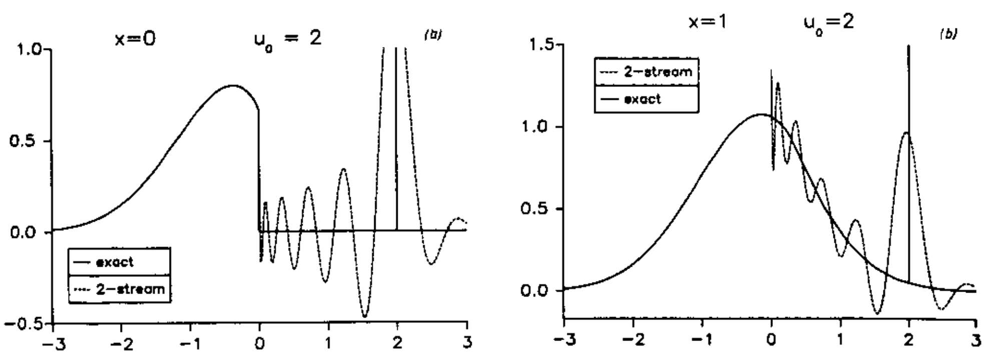

Figure 2. (a) The albedo solution $f(u,x)$ for an input velocity $u_0^{-1}\delta(u-u_0)$ with $u_0=2$, at $x=0$, as calculated using the exact expression (full curve) and the $N=28$ two-stream moment method (broken curve). For $u<0$ the two curves coincide on the scale of the figure. The delta function at $u=2$ is represented by a vertical bar. (b) The same quantities as in (a) for $x=1$.

To conclude this section, we note that the results for $A_0=n(\infty)$ and $n(0)$, given in (3.20) and (3.22), confirm the qualitative results obtained in [6] for the density profile in albedo problems: for subthermal injection ($u_0<1$) the density is larger than the corresponding equilibrium density in the boundary layer, but becomes smaller far from the wall (since the probability of a rapid return to the wall is large); for superthermal injection ($u_0>1$) the situation is reversed. For the Klein–Kramers case the situation is the same, as shown in figure 4 of [9]. The expression (3.22) allows us to calculate $n(0)$ for general $g(u)$ without solving the full albedo problem.

Table 2. The density at infinity $n^{\mathrm{A}}(\infty)$, the density at the wall $n^{\mathrm{A}}(0)$ and the limit $f^{\mathrm{A}}(-\varepsilon, 0)$ of the distribution function for $\varepsilon \downarrow 0$ for the albedo solution with input distribution $u_0^{-1}\delta(u-u_0)$ for several values of u_0, as calculated in the two-stream method in $N=28$ approximation ($2N$), as extrapolated to $N=\infty$ using the techniques of [6] (2∞), and by evaluation of the exact solution (ex). A dash in the rows (2∞) means that no reliable extrapolation could be made.

u_0		$n^{\mathrm{A}}(\infty)$	$n^{\mathrm{A}}(0)$	$f^{\mathrm{A}}(-0, x=0)$
0.01	($2N$)	1.024 758 07	102.6026	26.8318
	(2∞)	1.0259	102.59	—
	(ex)	1.025 960 98	102.5961	40.9299
0.1	($2N$)	1.179 740 12	11.800 332	4.766 96
	(2∞)	1.1797	11.799	4.74
	(ex)	1.179 819 05	11.798 191	4.706 79
1	($2N$)	2.248 352 28	2.248 3311	0.900 50
	(2∞)	2.248 351	2.248 35	0.90
	(ex)	2.248 351 18	2.248 3512	0.896 96
4	($2N$)	5.354 379 10	1.338 6312	0.536 23
	(2∞)	5.354 379	1.3386	0.53
	(ex)	5.354 378 44	1.338 5946	0.534 02
6	($2N$)	7.376 218 28	1.231 2331	0.528 57
	(2∞)	7.376 2	1.229	0.5
	(ex)	7.376 307 14	1.229 3845	0.490 45
8	($2N$)	9.421 653 28	0.495 7993	−16.1442
	(2∞)	—	—	—
	(ex)	9.388 970 56	1.173 6213	0.468 21

4. Partially reflecting boundaries

In the problems discussed in the preceding section all particles arriving at the wall are absorbed (or transmitted). This is not the most general case: when some of the particles arriving with velocity u' are reflected with velocity u, the boundary condition at $x=0$ takes the general form

$$uf(u,0)=\int_{-\infty}^{0}\mathrm{d}u'|u'|\sigma(u\mid u')f(u',0) \qquad \text{for } u>0. \tag{4.1}$$

The coefficients A_0 and $A(\lambda)$ in (3.1) are now no longer expressible by means of quadratures; instead they must be determined by solving an integral equation. We shall discuss this integral equation for the special case of partial specular reflection, $\sigma(u\mid u')=r\delta(u+u')$, for which we have

$$f^{r}(u,0)=rf^{r}(-u,0) \qquad \text{for } u>0. \tag{4.2}$$

In this case the Milne problem ($A_1^r=1$) leads to

$$\phi_0(u)\left\{A_0^r(1-r)-u(1+r)+P\int_0^{\infty}\mathrm{d}\lambda\, A^r(\lambda)[g_\lambda(u)-rg_\lambda(-u)]\right\}=0 \qquad \text{for } u>0. \tag{4.3}$$

By decomposing this equation with respect to the set (2.13), which is complete on the positive half-line, we obtain

$$A_0^r \equiv x_M^r = \frac{1}{1-r}\left[(1+r)x_M^{BGK} + r\int_0^\infty d\lambda \frac{\lambda A^r(\lambda)}{Q(\lambda)}\right] \tag{4.4}$$

where we used (3.6) and (2.17a), and the regular integral equation

$$A^r(\lambda) = \frac{-\lambda(1+r)}{C(\lambda)Q(\lambda)} + \frac{r\lambda}{C(\lambda)Q(\lambda)}\int_0^\infty dt\, K(t,\lambda)A^r(t) \tag{4.5a}$$

$$K(t,\lambda) = \frac{1}{\lambda}\left(\frac{t}{t+u}, g_\lambda\right)_+ = \frac{tp(\lambda)w(\lambda)}{(t+\lambda)\lambda} + tP\int_0^\infty \frac{du\, w(u)}{(t+u)(\lambda-u)} \tag{4.5b}$$

where we used (3.6) to determine the inhomogeneous term in (4.5a). The behaviour of the kernel $K(t,\lambda)$ for small and large t follows from (2.18) and (2.19a):

$$K(t,\lambda) \sim t/\lambda \text{ (small } t) \qquad K(t,\lambda) \sim t^{-1} \text{ (large } t). \tag{4.6}$$

At $t=\lambda=0$ the kernel is non-analytic, as is clear from

$$K(t,0) = 1 + \frac{t}{\sqrt{2\pi}}\ln t + \mathcal{O}(t) \tag{4.7}$$

which can be derived using the techniques from the appendix; the value $K(0,0)$ depends upon the direction from which the origin is approached, e.g. $\lim_{\varepsilon\downarrow 0} K(\varepsilon,\varepsilon) = \frac{1}{2}$.

A practical way to solve the integral equation (4.5a) is by expanding $A^r(t)$ in a suitable complete set of functions. We obtained good results by the expansion

$$A^r(t) = A^M(t)\sum_{n=0}^\infty b_n(r)\psi_{2n}(t) \qquad \psi_n = H_n(t\sqrt{2})/\sqrt{2^n n!} \tag{4.8}$$

with H_n the Hermite polynomials. This ansatz has the advantage that for $r=0$ the solution takes the simple form $b_n(0)=\delta_{n0}$. When this expression is substituted into (4.5a) and moments with respect to the odd Hermite functions $\phi_{2n+1}(\lambda) = \phi_0(\lambda)\psi_{2n+1}(\lambda)$ are taken, we obtain the set of linear equations

$$\sum_{m=0}^\infty [a_{2n+1,2m} + rg_{2n+1,2m}]b_m(r) = (1+r)a_{2n+1,0} \qquad n = 0, 1, 2, \ldots \tag{4.9a}$$

$$a_{nm} = \int_0^\infty d\lambda\, \phi_n(\lambda)\psi_m(\lambda) \tag{4.9b}$$

$$g_{nm} = \int_0^\infty d\lambda \int_0^\infty dt\, \phi_n(\lambda)K(t,\lambda)A^M(t)\psi_m(t). \tag{4.9c}$$

For practical calculations, the infinite set of equations (4.9a) must be truncated by the prescription $0 \leq m, n \leq N-1$. As is clear from table 3, already the $N=1$ approximation gives a good approximation to the quantities

$$x_M^r = A_0^r \qquad n^r(0) = A_0^r + \int_0^\infty d\lambda\, A^r(\lambda). \tag{4.10}$$

The 'mixed' representation (4.9) gives results that converge better than analogous representations obtained by taking moments with respect to even $\phi_n(\lambda)$ (or by expanding in odd $\psi_n(u)$); this may be due to the odd character of $K(t,\lambda)$, evident from (4.6).

Table 3. The Milne length x_M^r and the density at the wall $n^r(0)$ for the Milne problem with partial reflection, as calculated for various values of the reflection coefficient r by extrapolation of the two-stream method of [6] to $N=\infty$ (2∞), by solution of the integral equation (4.5) with an approximation of the sum in (4.8) by a single term (IE1) and by twelve terms (IE12).

r		x_M^r	$n^r(0)$
0.01	(2∞)	1.464 407 0973	1.022 503 3903
	(IE1)	1.464 407 04	1.022 585
	(IE12)	1.464 407 10	1.022 527
0.5	(2∞)	4.046 334 151	3.357 958 369
	(IE1)	4.045 93	3.364
	(IE12)	4.046 39	3.359
0.99	(2∞)	249.804 661 611	248.844 710 41
	(IE1)	249.71	248.77
	(IE12)	249.82	248.86

The results obtained by taking $N=12$ agree well with the results of the two-stream method, as is also clear from table 3. The accuracy reached is much less than that of the two-stream method, since the occurrence of multiple numerical integrations compels us to calculate $K(t, \lambda)$ merely in a discrete set of points, between which we must use interpolations.

The structure of the solution near the singularity can be determined by applying the techniques described in the appendix to the integral equation (4.3). The result is

$$A^r(\lambda)=\frac{r-1}{\sqrt{2\pi}}n^r(0)\left\{1+\frac{1+r}{\sqrt{2\pi}}\lambda\ln\lambda\right\}+\mathcal{O}(\lambda) \tag{4.11}$$

from which we find

$$f^r(-u,0)=\frac{n^r(0)}{\sqrt{2\pi}}\left\{1-\frac{1-r}{\sqrt{2\pi}}u\ln u\right\}+\mathcal{O}(u) \qquad \text{for } u>0 \tag{4.12a}$$

$$f^r(+u,0)=rf^r(-u,0). \tag{4.12b}$$

This result was quoted as (5.4) in [6].

5. Concluding remarks

The results described in this paper show that the singular eigenfunction method for solving kinetic boundary layer problems for the BGK equation can be used to obtain precise results for the distribution function. For problems that can be treated with the two-stream moment method the results of the two methods agree, but the two-stream method is much less time consuming and often more accurate; hence in practice the eigenfunction method should mainly be used for questions and problems for which the two-stream method is less suited, such as the determination of the exact analytical nature of singularities, or albedo problems with highly singular input distributions when the distribution function at the input side is of interest.

In the present paper we confined ourselves to the simplest version of the BGK equation. However, the methods used can be extended straightforwardly to somewhat more general problems. The restriction to one component of the velocity is not crucial: in more general problems a distribution function depending on one space variable only can be decomposed according to

$$f(\boldsymbol{u}, x) = \sum_{l=0}^{\infty} f_l(u_x, x)\chi_l(u_y, u_z) \tag{5.1}$$

with suitably chosen $\chi_l(u_y, u_z)$, and we obtain a set of equations like those treated in this paper for the f_l (with the second term on the right-hand side missing in (2.1) for $l>0$). The equations decouple for the pure Milne and albedo problems, but may be coupled for some problems with partial diffuse reflection. Other straightforward generalizations involve the full linear BGK equation [4], with a 5D null space of the collision operator, and the Laplace transform of the time-dependent BGK equation. Since in most problems involving these generalizations the two-stream moment method can also be used, and requires much less analytic and numerical effort, we shall not discuss the required modifications of the singular eigenfunction method, which are also treated extensively in the literature [3, 4, 11, 12], in any more detail.

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Appendix

In this appendix we first consider integrals of the type

$$I_1(f, \beta) = \int_0^{\infty} \mathrm{d}t\, f(t)\, \mathrm{e}^{-\beta/t} \tag{A.1}$$

$$I_2(f, \beta) = \int_0^{\infty} \mathrm{d}t\, f(t)(t+\beta)^{-1} \tag{A.2}$$

$$I_3(f, \beta) = \int_0^{\infty} \mathrm{d}t\, f(t) \ln(t+\beta) \tag{A.3}$$

which occur repeatedly in this paper, in the limit $\beta\downarrow 0$. All show a logarithmic dependence on β, with a coefficient determined by the limiting behaviour of $f(t)$ for low t. As an example, we consider the integral

$$I_{1,\varepsilon} = \int_0^{\varepsilon} \mathrm{d}t\, t^n\, \mathrm{e}^{-\beta/t} \approx \beta^{n+1} \int_{\beta/\varepsilon}^{\infty} \mathrm{d}y\, \mathrm{e}^{-y} y^{-n-2} \qquad \text{for } \beta \ll \varepsilon \ll 1 \tag{A.4}$$

for which one finds, using 3.351.4 of [14],

$$I_{1,\varepsilon} = \frac{(-1)^{n+1}\beta^{n+1}}{(n+1)!}\Gamma(0, \beta/\varepsilon) + \mathrm{e}^{-\beta/\varepsilon} \sum_{k=0}^{n} \frac{(-1)^k \beta^k \varepsilon^{n+1-k}}{(n+1)\ldots(n+1-k)} \tag{A.5}$$

where $\Gamma(a, x)$ is the incomplete Γ-function, [14], section 8.35, which for small arguments has the representation

$$\Gamma(0, \beta/\varepsilon) = -c_{\mathrm{E}} - \ln\beta + \ln\varepsilon - \sum_{k=1}^{\infty} \frac{(-1)^k(\beta/\varepsilon)^k}{k\cdot k!} \tag{A.6}$$

where c_E is Euler's constant. We see that the leading singular term has a coefficient independent of ε. Hence we find

$$I_1(f,\beta)=I_1(f,0)+a\frac{(-1)^n\beta^{n+1}}{(n+1)!}\ln\beta+\mathcal{O}(\beta^k,k>0) \qquad \text{if } f(t)\approx at^n \text{ for small } t. \tag{A.7}$$

Similarly, the asymptotic behaviour of $I_2(f)$ can be extracted from the integral 3.383.10 of [14]

$$\begin{aligned}I_{2,\mu}&=\int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\mu t}t^{\alpha+1}(t+\beta)^{-1}\\&=\beta^{\alpha+1}\,\mathrm{e}^{\beta\mu}\Gamma(\alpha+2)\Gamma(-1-\alpha,\beta\mu)\end{aligned} \tag{A.8}$$

which for integer α has a leading logarithmic singularity independent of μ. Hence we find

$$I_2(f,\beta)\approx I_2(f,0)+a(-1)^{n+1}\beta^n\ln\beta \qquad \text{if } f(t)\approx at^n \tag{A.9}$$

where the singularity is caused by $\Gamma(-n,x)$ for integer n. By differentiating $I_{2\mu}$ with respect to α and subsequently choosing α to be the integer we obtain

$$I_2(f,\beta)\approx I_2(f,0)+(a/2)(-1)^{n+1}\beta^n\ln^2\beta \qquad \text{if } f(t)\approx at^n\ln t. \tag{A.10}$$

By using the relation

$$I_2(f,\beta)=\frac{\partial}{\partial\beta}I_3(f,\beta) \tag{A.11}$$

we arrive at the relations

$$I_3(f,\beta)\approx I_3(f,0)+\frac{a(-1)^{n+1}}{n+1}\beta^{n+1}\ln\beta \qquad \text{for } f(t)\approx at^n \tag{A.12}$$

and

$$I_3(f,\beta)\approx I_3(f,0)+\frac{a(-1)^{n+1}\beta^{n+1}}{n+1}\left[\frac{\ln^2\beta}{2}-\frac{\ln\beta}{n+1}\right]$$
$$\text{for } f(t)\approx at^n\ln t. \tag{A.13}$$

The correction terms specified in (A.8)–(A.13) are always the largest *singular* terms; for $n>0$ there may be terms analytic in β that are of lower order in β (β, β^2, etc).

The estimate (A.12) is used in evaluating (2.10b) for $Q(\lambda)$, with the result (2.23a), and $A^{\mathrm{M}}(\lambda)$ in (3.6). The estimates (A.7) and (A.9) are used for analysing the singularity in $f^{\mathrm{M}}(u,x)$ near $u=x=0$; their main use is in showing that the terms neglected in the transition from (3.10) to (3.11), or from (3.12) to (3.13), are of order $u\ln u$, and hence negligible relative to the orders retained. In some classes, the integrals contain more than one of the factors considered in (A.1)–(A.3); it is clear, however, that the correction terms can simply be added for small β, provided the exponent n in (A.7)–(A.13) is non-negative. The singularity for integrals of type

$$I_4(f,\beta)=P\int_0^\infty \mathrm{d}t\,f(-t)(t-\beta)^{-1} \tag{A.14}$$

is similar to that of I_2, at least for $f(t)$ that are differentiable at $t=0$, since

$$I_4-I_2=P\int_{-\infty}^{+\infty}\mathrm{d}t\frac{f(-t)}{t-\beta}=P\int_{-\infty}^{+\infty}\mathrm{d}t\frac{f(-t-\beta)}{t} \tag{A.15}$$

is analytic in β for such $f(t)$. Estimates of type (A.9) enter, for example, into the estimate (4.7).

The second problem considered in this appendix is the treatment of the distribution (3.23), when appearing inside of integrals such as that in (3.21). Since the regular part of $f(u,x)$ was already determined in the text leading up to (3.25), we merely need to determine the coefficient of $\delta(\lambda-u)\delta(\lambda-u_0)$, which leads to the $\delta(u-u_0)$ term in (3.25). To that purpose we use the representations

$$P\frac{1}{\lambda-u}=\lim_{\varepsilon\downarrow 0}\left[\frac{1}{\lambda-u+\mathrm{i}\varepsilon}+\mathrm{i}\pi\delta(\lambda-u)\right] \tag{A.15a}$$

$$P\frac{1}{\lambda-u_0}=\lim_{\varepsilon\downarrow 0}\left[\frac{1}{\lambda-u_0-\mathrm{i}\varepsilon}-\mathrm{i}\pi\delta(\lambda-u_0)\right]. \tag{A.15b}$$

Substitution into (3.23) and (3.21) gives a contribution of type $\delta(u-u_0)$ resulting from $\delta(\lambda-u)\delta(\lambda-u_0)$ in the integrand, with a coefficient equal to

$$\mathrm{e}^{-x/u}\frac{\Phi_0(u_0)Q(u_0)[\pi^2u_0^2+p^2(u_0)]}{C(u_0)Q(u_0)}=\frac{\mathrm{e}^{-x/u_0}}{u_0} \tag{A.16}$$

where we used (2.10c). This confirms the conjecture in (3.25). The remaining terms give rise to regular contributions; for integral expressions involving the distribution (3.23) we thus find

$$\begin{aligned} P\int_0^\infty \mathrm{d}\lambda\, f(\lambda)g_\lambda(u)g_\lambda(u_0) &\sim \frac{\partial}{\partial u_0}P\int_0^\infty \mathrm{d}\lambda\,\lambda f(\lambda)g_\lambda(u_0) \\ &\quad+\frac{C(u_0)}{u_0\phi_0(u_0)}f(u_0)\delta(u-u_0) \qquad \text{for } u\to u_0 \end{aligned} \tag{A.17}$$

for sufficiently smooth $f(\lambda)$. For the special case $f(\lambda)=[C(\lambda)Q(\lambda)]^{-1}$ we recover from (A.17) the completeness relation (2.12). The agreement shown in figure 2 between the expression calculated by (3.25) and the result obtained by the two-stream method serves as an additional check on the derivation sketched above.

References

[1] Bhatnagar P L, Gross E P and Krook M 1954 *Phys. Rev.* **94** 511
[2] Welander P 1954 *Ark. Fys.* 7 507
[3] Case K M and Zweifel P F 1967 *Linear Transport Theory* (Reading: Addison-Wesley)
[4] Cercignani C 1988 *The Boltzmann Equation and its Applications* (Berlin: Springer)
[5] Widder M E and Titulaer U M 1989 *J. Stat. Phys.* **56** 471
[6] Kainz A J and Titulaer U M 1992 *J. Phys. A: Math. Gen.* **25** 1855
[7] Klein O 1922 *Ark. Mat. Astron. Fys.* **16**(5) 1
Kramers H A 1940 *Physica* **7** 284
[8] Marshall T W and Watson E J 1985 *J. Phys. A: Math. Gen.* **18** 3531
Duck P W, Marshall T W and Watson E J 1986 *J. Phys. A: Math. Gen.* **19** 3545
Marshall T W and Watson E J 1987 *J. Phys. A: Math. Gen.* **20** 1345
[9] Kainz A J and Titulaer U M 1991 *J. Phys. A: Math. Gen.* **24** 4677
[10] Van Kampen N G 1955 *Physica* **21** 949
[11] Case K M 1960 *Ann. Phys., NY* **9** 1
[12] Duderstadt J J and Martin W R 1978 *Transport Theory* (New York: Wiley)
[13] Kuscer I and McCormick N J 1973 *Adv. Nucl. Sci.* **7** 181
[14] Gradshteyn I S and Ryzhik I M 1980 *Table of Integrals, Series and Products* (San Diego: Academic)