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Kramers' problem for a variable collision frequency model

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The often-studied problem known as Kramers' problem, in the general area of rarefied-gas dynamics, is investigated in terms of a linearized, variable collision frequency model of the Boltzmann equation. A convenient change of variables is used to reduce the general case considered to a canonical form that is well suited for analysis by analytical and/or numerical methods. While the general formulation developed is valid for an unspecified collision frequency, a recently developed version of the discrete-ordinates method is used to compute the viscous-slip coefficient and the velocity defect in the Knudsen layer for three specific cases: the classical BGK model, the Williams model (the collision frequency is proportional to the magnitude of the velocity) and the rigid-sphere model.

1 Introduction

It is generally considered by workers in the area of rarefied-gas dynamics/kinetic theory that Kramers' problem is the most basic way that we can see the effect of a wall or boundary on the flow of gas particles. For this problem a collection of gas particles (in a semi-infinite medium) flows past a fixed boundary (wall) in such a way that the z-component (parallel to the plane boundary) of the velocity is linear in the variable x that measures the distance from the wall. We consider that Kramers' problem is the simplest of a general class of problems in kinetic theory, but it is the problem most often investigated since we are able to see the effect of the wall on the flow (thus defining the Knudsen layer) without some of the additional complications that other more realistic problems, such as flow in a plane channel or cylindrical tube, would introduce.

Here, following the basic books of Cercignani [1,2] and Williams [3], we consider that the diffusion of gas particles as they flow past a flat plate can be described mathematically by the Boltzmann equation. For the general case the gas particles interact with each other according to some inter-atomic force laws, and these same particles interact with the wall according to specified reflection laws. So it is clear that, unless some special conditions are specified, the scattering term in the Boltzmann equation will depend on the particle distribution function in a nonlinear way. We note that Monte Carlo methods and computationally intensive iterative methods, for example, are ways of attempting to extract some physical information from the nonlinear Boltzmann equation. Another approach that can be used when the density of particles is small (rarefied-gas dynamics) is to replace the nonlinear Boltzmann equation by a so-called model equation. While the most widely used model equation is the BGK model introduced by Bhatnagar, Gross

& Krook [4], there has been also considerable interest [5–10] in the variable collision frequency model of the Boltzmann equation since this model has been shown [8] better able to support some experimental observations.

In this work we make use of the transformations used by Busbridge [11] and Bednarz & Mika [12] to reformulate our basic problem in a form that we are well able to solve numerically in terms of a recently reported version [13] of the discrete-ordinates method [14]. We thus consider this work to be firstly a review of the use of the transformations used by Busbridge [11] and Bednarz & Mika [12] for a general version of Kramers' problem and secondly to be another implementation of our version [13] of the discrete-ordinates method. In this way we are able to obtain, in a concise and accurate way, numerical results for the viscous-slip coefficient and the velocity defect for three special cases relevant to the variable collision frequency model of the Boltzmann equation, *viz.* the classical BGK model, the Williams model (the collision frequency is proportional to the magnitude of the velocity) and the rigid-sphere model. Also since our discrete-ordinates method works well with general boundary conditions, we are able to evaluate the effects of specular reflection by the wall.

We choose to start our work with the developed formulation of the Kramers problem as given by Williams [3]. We therefore consider the defining balance equation to be

$$S(c,\mu) + c\mu\frac{\partial}{\partial x}g(x,c,\mu) + V(c)g(x,c,\mu) = \int_0^\infty \int_{-1}^1 K(c',\mu' : c,\mu)g(x,c',\mu')\,\mathrm{d}\mu'\,\mathrm{d}c', \tag{1}$$

where

$$S(c,\mu) = 2K_0c^2\mu(1-\mu^2)^{1/2} \tag{2}$$

and

$$K(c',\mu' : c,\mu) = \frac{1}{4}\gamma_1 cc'^3 V(c)V(c')(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}\mathrm{e}^{-c'^2}. \tag{3}$$

Here

$$\gamma_1 = \frac{3}{V_2} \quad \text{with} \quad V_2 = \int_0^\infty c^4 V(c)\mathrm{e}^{-c^2}\,\mathrm{d}c. \tag{4a,b}$$

In addition, c is used, with dimensionless units, to denote the magnitude of the particle velocity vector $\boldsymbol{c}$, x (also in dimensionless units) is the spatial variable that measures the distance from the wall, $V(c)$ is the collision frequency and μ is the cosine of the angle between the velocity vector and the (positive) x axis. For the Kramers problem it is assumed that the z-component (parallel to the plate) of the net velocity $q_z(x)$ is constant with respect to the spatial variable z. But at the same time $q_z(x) \sim K_0 x$ as $x \to \infty$, so, as discussed by Williams [3,15], there exists in Eq. (1) the inhomogeneous term given by Eq. (2). In regard to the dependent variable $g(x,c,\mu)$ in Eq. (1), we note that Williams [3,15], in the process of linearizing the nonlinear Boltzmann equation, expressed the particle distribution function $f(\boldsymbol{r},\boldsymbol{c})$ in the form

$$f(\boldsymbol{r},\boldsymbol{c}) = f_0(\boldsymbol{r},\boldsymbol{c})[1+h(\boldsymbol{r},\boldsymbol{c})], \tag{5}$$

where $f_0(\boldsymbol{r},\boldsymbol{c})$ would be the distribution of gas particles were it not for the presence of the wall. Upon considering that our problem depends on only one spatial variable x, writing the velocity vector in polar coordinates c, $\cos^{-1}\mu$ and ϕ and defining

$$g(x,c,\mu) = \frac{1}{\pi}\int_0^{2\pi} h(x,c,\mu,\phi)\cos\phi\,\mathrm{d}\phi, \tag{6}$$

Williams finds Eq. (1) and the boundary condition

$$g(0,c,\mu) = (1-\alpha)g(0,c,-\mu) \tag{7}$$

for $\mu \in (0,1]$ and all c. For the considered formulation, the wall reflects particles with a mixture, measured by the accommodation coefficient α, of diffuse and specular components; however, because of the azimuthal average used in Eq. (6), we see in Eq. (7) only the specular component.

Having defined the basic elements of the Kramers problem considered here, we intend to establish a solution (bounded as x tends to infinity) of Eq. (1) that satisfies the boundary condition given as Eq. (7). While we will define the complete solution $g(x,c,\mu)$, our numerical work is aimed at computing the velocity profile

$$q_z(x) = K_0 x + \pi^{-1/2}\int_0^{\infty}\int_{-1}^{1} c^3 \mathrm{e}^{-c^2}(1-\mu^2)^{1/2} g(x,c,\mu)\,\mathrm{d}\mu\,\mathrm{d}c \tag{8}$$

that is the principal quantity of interest [3,15]. We note that in formulating this version of the Kramers problem we have made much use of the notation and development given in Refs. [3] and [15]; however, the papers of Cercignani [6] and Loyalka & Ferziger [7] are the ones we consider to be the defining works on this subject of the variable collision frequency model of the linearized Boltzmann equation. It therefore seems reasonable to refer to the general model equation used in this work as the CLF equation and to consider the BGK model, the Williams model and the rigid-sphere model as special cases that correspond to certain choices of the collision frequency $V(c)$. While the basic elements of the solution developed are valid for a general collision frequency, the numerical work reported here is based on three special cases (the BGK model, the Williams model and the rigid-sphere model). And so to be very clear about the terminology we use, we note that we consider the classical BGK model to be defined by a constant collision frequency. For the Williams model the collision frequency is proportional to the magnitude of the velocity, and for the rigid-sphere model the collision frequency is (as will be seen) expressed in terms of the error function and other elementary functions.

2 A reformulation

To begin a transformation of the considered problem to form more convenient for analytical or numerical work, we first note that

$$g_p(c,\mu) = -\frac{S(c,\mu)}{V(c)} \tag{9}$$

is a particular solution of Eq. (1), and so we write

$$g(x,c,\mu) = g_h(x,c,\mu) + g_p(c,\mu), \tag{10}$$

where $g_h(x, c, \mu)$ must satisfy

$$c\mu \frac{\partial}{\partial x} g_h(x, c, \mu) + V(c) g_h(x, c, \mu) = \int_0^\infty \int_{-1}^1 K(c', \mu' : c, \mu) g_h(x, c', \mu') \, \mathrm{d}\mu' \, \mathrm{d}c' \tag{11}$$

and the boundary condition

$$g_h(0, c, \mu) - (1 - \alpha) g_h(0, c, -\mu) = \frac{2}{V(c)} (2 - \alpha) K_0 \mu (1 - \mu^2)^{1/2} c^2 \tag{12}$$

for $\mu \in (0, 1]$ and all c. Continuing, we let

$$g_h(x, c, \mu) = c(1 - \mu^2)^{1/2} Y(x, c, \mu) \tag{13}$$

to obtain

$$c\mu \frac{\partial}{\partial x} Y(x, c, \mu) + V(c) Y(x, c, \mu) = \frac{1}{4} \gamma_1 V(c) \int_0^\infty \int_{-1}^1 c'^4 \mathrm{e}^{-c'^2} V(c') (1 - \mu'^2) Y(x, c', \mu') \, \mathrm{d}\mu' \, \mathrm{d}c' \tag{14}$$

and the boundary condition

$$Y(0, c, \mu) - (1 - \alpha) Y(0, c, -\mu) = \frac{2}{V(c)} (2 - \alpha) K_0 c \mu \tag{15}$$

for $\mu \in (0, 1]$ and all c. We now let

$$V(c) = \sigma \eta(c), \quad \tau = \sigma x \quad \text{and} \quad \varpi = \frac{\sigma}{4} \gamma_1 \tag{16a, b, c}$$

and rewrite Eq. (14) as

$$c\mu \frac{\partial}{\partial \tau} Y(\tau/\sigma, c, \mu) + \eta(c) Y(\tau/\sigma, c, \mu) = \varpi \eta(c) \int_0^\infty \int_{-1}^1 c'^4 \mathrm{e}^{-c'^2} \eta(c') (1 - \mu'^2) Y(\tau/\sigma, c', \mu') \, \mathrm{d}\mu' \, \mathrm{d}c'. \tag{17}$$

At this point we consider the constant σ to be a scale factor that can be useful for normalizing the collision frequency $V(c)$. Of course, τ now is our renormalized spatial variable, and

$$\varpi = \frac{3}{4\eta_4}, \quad \text{with} \quad \eta_4 = \int_0^\infty c^4 \eta(c) \mathrm{e}^{-c^2} \, \mathrm{d}c, \tag{18a, b}$$

clearly depends only on the shape factor $\eta(c)$. Finally, we follow the work of Busbridge [11] and Bednarz & Mika [12] and make use of the transformations

$$\xi = c\mu/\eta(c) \quad \text{and} \quad Y[\tau/\sigma, c, \xi\eta(c)/c] = \frac{2K_0}{\sigma} G(\tau, \xi) \tag{19a, b}$$

to rewrite Eq. (17), after an interchange of orders of integration, as

$$\xi \frac{\partial}{\partial \tau} G(\tau, \xi) + G(\tau, \xi) = \varpi \int_{-\gamma}^{\gamma} \int_{M_{\xi'}} c' \mathrm{e}^{-c'^2} \eta^2(c') [c'^2 - \xi'^2 \eta^2(c')] G(\tau, \xi') \, \mathrm{d}c' \, \mathrm{d}\xi', \tag{20}$$

where

$$\gamma = \sup\{c/\eta(c)\} \tag{21}$$

and

$$c \in M_\xi \quad \text{if} \quad \frac{\eta(c)|\xi|}{c} \leqslant 1. \tag{22}$$

We now define

$$\Psi(\xi) = \varpi \int_{M_\xi} c\eta^2(c)[c^2 - \xi^2\eta^2(c)]\mathrm{e}^{-c^2}\,\mathrm{d}c \tag{23}$$

and write Eq. (20) as

$$\xi \frac{\partial}{\partial \tau} G(\tau, \xi) + G(\tau, \xi) = \int_{-\gamma}^{\gamma} \Psi(\xi')G(\tau, \xi')\,\mathrm{d}\xi'. \tag{24}$$

It follows, since $g(\tau/\sigma, c, \mu)$ must be bounded as τ tends to infinity, that we must seek a similarly bounded solution of Eq. (24) that also satisfies the boundary condition

$$G(0, \xi) - (1 - \alpha)G(0, -\xi) = (2 - \alpha)\xi, \quad \xi \in (0, \gamma]. \tag{25}$$

Now, looking back to Eq. (8), we find we can express the desired velocity profile in terms of the solution to our 'G problem.' Thus

$$q_z(x) = K_0 q(x), \tag{26}$$

where

$$q(x) = x + \frac{1}{\sigma}\int_{-\gamma}^{\gamma} \psi(\xi)G(\sigma x, \xi)\,\mathrm{d}\xi \tag{27}$$

and

$$\psi(\xi) = 2\pi^{-1/2} \int_{M_\xi} c\eta(c)[c^2 - \xi^2\eta^2(c)]\mathrm{e}^{-c^2}\,\mathrm{d}c. \tag{28}$$

It is clear that the scale factor σ will have a fundamental effect on our reported numerical results, and, since there already exist many inconsistencies in the literature concerning the definition of an appropriate scale factor, we elect here to use one of Loyalka's choices [8], and so we define

$$\sigma = \frac{16}{15}\pi^{-1/2} \int_0^{\infty} \eta^{-1}(c)c^6\mathrm{e}^{-c^2}\,\mathrm{d}c \tag{29}$$

for all models we consider. To complete this section we let

$$\lim_{\tau \to \infty} G(\tau, \xi) = G(\infty, \xi) \tag{30}$$

and

$$q_{\mathrm{asy}}(x) = x + \frac{1}{\sigma}\int_{-\gamma}^{\gamma} \psi(\xi)G(\infty, \xi)\,\mathrm{d}\xi, \tag{31}$$

and so the viscous slip coefficient defined by

$$q_{\mathrm{asy}}(-\zeta) = 0 \tag{32}$$

is given as

$$\zeta = \frac{1}{\sigma}\int_{-\gamma}^{\gamma} \psi(\xi)G(\infty, \xi)\,\mathrm{d}\xi. \tag{33}$$

In this work we compute the velocity profile $q(x)$, but we will present this quantity more effectively by tabulating for various cases the viscous-slip coefficient ζ and the velocity defect

$$q_{\mathrm{d}}(x) = q_{\mathrm{asy}}(x) - q(x). \tag{34}$$

3 Three special cases

We intend to implement our solution numerically for three special cases, and so now we note the relevant forms of certain basic quantities we require. Our first special case is the classical BGK model for which we write $\eta(c) = 1$ and find, from Eqs. (21), (23), (28) and (29), $\gamma = \infty$ and $\sigma = 1$ along with

$$\Psi(\xi) = \psi(\xi) = \pi^{-1/2} \mathrm{e}^{-\xi^2}. \tag{35}$$

Continuing, we take our second special case to be the Williams model for which $\eta(c) = c$ and for which we find, again from Eqs. (21), (23), (28) and (29), $\gamma = 1$,

$$\sigma = \frac{16}{15} \pi^{-1/2} \tag{36}$$

and

$$\Psi(\xi) = \psi(\xi) = \frac{3}{4}(1 - \xi^2). \tag{37}$$

Our third special case, the rigid-sphere model, is defined by

$$\eta(c) = \left(2c + \frac{1}{c}\right) \frac{\pi^{1/2}}{2} \mathrm{erf}(c) + \mathrm{e}^{-c^2}, \tag{38}$$

where $\mathrm{erf}(c)$ is the error function. Here we can easily show that $\gamma = \pi^{-1/2}$ and from Eqs. (18) that

$$\varpi = \frac{3}{7} \left(\frac{2}{\pi}\right)^{1/2}. \tag{39}$$

However, in regard to Eqs. (23), (28) and (29) we have not found explicit results and so must use numerical methods to define $\Psi(\xi)$ and $\psi(\xi)$ and σ for this case. We have used the MAPLE V software to evaluate the integral in Eq. (29) numerically, and so in this way we found, for this case,

$$\sigma = 0.278804052827\ldots. \tag{40}$$

At this point we must consider Eq. (22) in order to define the required functions $\Psi(\xi)$ and $\psi(\xi)$. We let

$$f(c) = \frac{c}{\eta(c)}, \tag{41}$$

and note that we can show, for the case considered, that $f'(c) > 0$, for $c \geqslant 0$ and so the inverse function

$$m(\xi) = f^{-1}(|\xi|), \quad \xi \in [-\gamma, \gamma], \tag{42}$$

exists, and thus we can write

$$\Psi(\xi) = \varpi \int_{m(\xi)}^{\infty} c\eta^2(c)[c^2 - \xi^2\eta^2(c)]\mathrm{e}^{-c^2}\,\mathrm{d}c \tag{43}$$

and

$$\psi(\xi) = \frac{2}{\pi^{1/2}} \int_{m(\xi)}^{\infty} c\eta(c)[c^2 - \xi^2\eta^2(c)]\mathrm{e}^{-c^2}\,\mathrm{d}c \tag{44}$$

which can be evaluated numerically once $m(\xi)$ is available; in this work we use Newton's method to establish the required numerical values of $m(\xi)$.

4 A discrete-ordinates solution

While the use of the terminology 'discrete ordinates' is not common in the area of rarefied-gas dynamics, it has been in use for many years in the field of radiative transfer. In fact, it seems the most credit for the introduction and development of this method in the general area of particle transport theory should go to Chandrasekhar [14] who in his fundamental work on radiative transfer did much to define the method as an effective computational tool. The method as used by Chandrasekhar had, however, one difficult computational aspect that kept the method from being used effectively past a certain order. This practical limitation is due to the fact that the required 'separation constants' are defined in terms of the zeros of a certain polynomial. Since Chandrasekhar's work [14] there have been, naturally, numerous improvements in the method, and it has been shown, see for example Ref. [16], that under certain restrictions on the quadrature scheme, the discrete-ordinates method is equivalent to the spherical-harmonics method (often used in radiative transfer and neutron transport theory) and that the separation constants can be computed as the eigenvalues of a tridiagonal matrix – a much easier task than finding zeros of polynomials. Here in this work we use what we consider to be a modern version [13] of the discrete-ordinates method that (i) does not depend on any special properties of the quadrature scheme and (ii) has the separation constants defined as the eigenvalues of a matrix with special properties (diagonal matrix plus a rank-one update) so that the basic eigenvalue computation is of a type generally considered even easier than the one for a tridiagonal matrix. We note that the variation of the discrete ordinates method used here has already been successfully used [17–21] in the area of radiative transfer to solve, for example, most of Chandrasekhar's basic problems (for very high-order anisotropic scattering and including all polarization effects), a non coherent scattering model (that also includes polarization effects), the classical searchlight problem and coupled radiation/conduction heat-transfer problems of engineering interest. In the field of kinetic theory the modeling process closest to the discrete-ordinates method we use is the discrete-velocity method [or Broadwell model] as discussed, for example, by Refs. [22–24]. As will be seen, however, the version of the discrete-ordinates method we develop here has some analytical aspects that make it, in our opinion, much more computationally efficient than what is normally achieved with discrete-velocity approximations.

The variation of the discrete-ordinates method [14] we use in this work was developed in Ref. [13], and so we can make use of that material now to solve our G problem that was formulated in Section 2. We thus approximate the integral term in Eq. (24) by a quadrature formula and write our discrete-ordinates equations as

$$\pm\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \pm\xi_i) + G(\tau, \pm\xi_i) = \sum_{k=1}^{N} w_k \Psi(\xi_k)[G(\tau, \xi_k) + G(\tau, -\xi_k)] \tag{45}$$

for $i = 1, 2, \ldots, N$. In writing Eq. (45) we have taken into account the fact that the 'characteristic function' $\Psi(\xi)$ is an even function. In addition, we clearly are considering that the N quadrature points $\{\xi_k\}$ and the N weights $\{w_k\}$ are defined for use on the integration interval $[0, \gamma]$. We note that it is to this feature of using a 'half-range' quadrature scheme that we partially attribute the especially good accuracy we have obtained from the solution reported here. Seeking exponential solutions, we substitute

$$G(\tau, \pm\xi_i) = \phi(v, \pm\xi_i)\mathrm{e}^{-\tau/v} \tag{46}$$

into Eq. (45) to find

$$\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_+ = (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{\Phi}_+ - \boldsymbol{W}\boldsymbol{\Phi}_- \tag{47a}$$

and

$$-\frac{1}{v}\boldsymbol{M}\boldsymbol{\Phi}_- = (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{\Phi}_- - \boldsymbol{W}\boldsymbol{\Phi}_+ \tag{47b}$$

where $\boldsymbol{I}$ is the $N \times N$ identity matrix,

$$\boldsymbol{\Phi}_\pm = \left[\phi(v, \pm\xi_1), \phi(v, \pm\xi_2), \ldots, \phi(v, \pm\xi_N)\right]^{\mathrm{T}}, \tag{48}$$

the superscript T denotes the transpose operation, the elements of the matrix $\boldsymbol{W}$ are

$$(\boldsymbol{W})_{i,j} = w_j \Psi(\xi_j), \tag{49}$$

and

$$\boldsymbol{M} = \mathrm{diag}\{\xi_1, \xi_2, \ldots, \xi_N\}. \tag{50}$$

If we now let

$$\boldsymbol{U} = \boldsymbol{\Phi}_+ + \boldsymbol{\Phi}_- \tag{51}$$

then we can eliminate between the sum and the difference of Eqs. (47) to find

$$(\boldsymbol{D} - 2\boldsymbol{M}^{-1}\boldsymbol{W}\boldsymbol{M}^{-1})\boldsymbol{M}\boldsymbol{U} = \frac{1}{v^2}\boldsymbol{M}\boldsymbol{U} \tag{52}$$

where

$$\boldsymbol{D} = \mathrm{diag}\{\xi_1^{-2}, \xi_2^{-2}, \ldots, \xi_N^{-2}\}. \tag{53}$$

Multiplying Eq. (52) by a diagonal matrix $\boldsymbol{T}$, we find

$$(\boldsymbol{D} - 2\boldsymbol{V})\boldsymbol{X} = \frac{1}{v^2}\boldsymbol{X} \tag{54}$$

where

$$\boldsymbol{V} = \boldsymbol{M}^{-1}\boldsymbol{T}\boldsymbol{W}\boldsymbol{T}^{-1}\boldsymbol{M}^{-1} \tag{55}$$

and

$$\boldsymbol{X} = \boldsymbol{T}\boldsymbol{M}\boldsymbol{U}. \tag{56}$$

As discussed in Ref. [13], we can define the elements $t_1, t_2, \dots, t_N$ of $\boldsymbol{T}$ so as to make $\boldsymbol{V}$ symmetric; and therefore, since $\boldsymbol{V}$ is a symmetric, rank-one matrix, we can write our eigenvalue problem in the form

$$(\boldsymbol{D} - 2\boldsymbol{z}\boldsymbol{z}^{\mathrm{T}})\boldsymbol{X} = \lambda \boldsymbol{X} \tag{57}$$

where $\lambda = 1/v^2$ and

$$\boldsymbol{z} = \Big[\{w_1 \Psi(\xi_1)\}^{1/2}/\xi_1, \{w_2 \Psi(\xi_2)\}^{1/2}/\xi_2, \dots, \{w_N \Psi(\xi_N)\}^{1/2}/\xi_N\Big]^{\mathrm{T}}. \tag{58}$$

We note that the eigenvalue problem defined by Eq. (57) is of a form that is encountered when the so-called 'divide and conquer' method [25] is used to find the eigenvalues of tridiagonal matrices. In addition, we see from Eq. (53) that, because of the way our basic eigenvalue problem is formulated, we must exclude zero from the set of quadrature points. Of course to exclude zero from the quadrature set is not considered a serious restriction since typical Gauss quadrature schemes do not include the end points of the integration interval.

Considering that we have found the required eigenvalues from Eq. (57), we impose the normalization condition

$$\sum_{k=1}^{N} w_k \Psi(\xi_k)[\phi(v, \xi_k) + \phi(v, -\xi_k)] = 1 \tag{59}$$

so that we can write our discrete-ordinates solution as

$$G(\tau, \pm\xi_i) = \sum_{j=1}^{N} \left(A_j \frac{v_j}{v_j \mp \xi_i} \mathrm{e}^{-\tau/v_j} + B_j \frac{v_j}{v_j \pm \xi_i} \mathrm{e}^{\tau/v_j} \right) \tag{60}$$

where the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the conditions placed on the solution, and where the separation constants $\{v_j\}$ are the reciprocals of the positive square roots of the eigenvalues defined by Eq. (57). It is clear from Eq. (60) that we cannot allow any separation constant to be equal to one of the quadrature points.

At this point we find it convenient to modify slightly the discrete-ordinates solution reported in Ref. [13]. We note that problems based on Eq. (24) are conservative since

$$\int_{-\gamma}^{\gamma} \Psi(\xi)\, \mathrm{d}\xi = 1, \tag{61}$$

and so we expect that one of the eigenvalues defined by Eq. (57) should tend to zero as N tends to infinity. We choose to take this fact into account by explicitly neglecting v_N, the largest of the computed separation constants $\{v_j\}$ and, subsequently, by writing Eq. (60) as

$$G(\tau, \pm\xi_i) = A + B(\tau \mp \xi_i) + \sum_{j=1}^{N-1} \left(A_j \frac{v_j}{v_j \mp \xi_i} \mathrm{e}^{-\tau/v_j} + B_j \frac{v_j}{v_j \pm \xi_i} \mathrm{e}^{\tau/v_j} \right). \tag{62}$$

Of course, the constants A, B, $\{A_j\}$ and $\{B_j\}$ that are present in Eq. (62) must now be fixed so that $G(\tau, \pm\xi_i)$ satisfies the condition at infinity and the boundary condition listed as Eq. (25). To keep $G(\tau, \pm\xi_i)$ bounded we set all the B coefficients to zero, and so we obtain

$$G(\tau, \pm\xi_i) = A + \sum_{j=1}^{N-1} A_j \frac{\nu_j}{\nu_j \mp \xi_i} e^{-\tau/\nu_j}. \tag{63}$$

Upon substituting Eq. (63) into Eq. (25) evaluated at the N quadrature points $\{\xi_k\}$ we obtain the $N \times N$ system of linear algebraic equations we solve to define the constants in Eq. (63). In this way the solution $G(\tau, \pm\xi_i)$ is established. Finally we use Eq. (63) in Eqs. (27) and (33) to obtain

$$q(x) = x + \frac{1}{\sigma}\left(A + \sum_{j=1}^{N-1} A_j N_j e^{-\sigma x/\nu_j}\right) \tag{64}$$

and

$$\zeta = \frac{A}{\sigma}, \tag{65}$$

where

$$N_j = 2\nu_j^2 \sum_{k=1}^{N} \psi(\xi_k) \frac{w_k}{\nu_j^2 - \xi_k^2}. \tag{66}$$

We note that in obtaining Eq. (64) we have integrated the first term in Eq. (63) analytically, but the defined quadrature scheme was used to integrate the remaining terms.

5 Numerical results

The first thing we must do is to define the quadrature scheme to be used in our discrete-ordinates solution, and, since we have considered three different cases, to which we refer as case 1, case 2 and case 3 while meaning respectively, the BGK model, the Williams model and the rigid-sphere model, we have used three different maps. For case 1, we used the transformation

$$u(\xi) = \exp\{-\xi\} \tag{67}$$

to map $\xi \in [0, \infty)$ into $u \in [0, 1]$, and we then used a Gauss-Legendre scheme mapped (linearly) onto the interval $[0, 1]$. For case 2 and case 3 we simply mapped the Gauss-Legendre scheme onto, respectively, the intervals $[0, 1]$ and $[0, \pi^{-1/2}]$.

Having defined our quadrature schemes and in developing a FORTRAN implementation of our solution, we found the required separation constants $\{\nu_j\}$ by using the special numerical package DZPACK [26] that was developed to take advantage of the special structure of Eq. (57) to solve our eigenvalue problem. The required separation constants were then available as the reciprocals of the positive square roots of these eigenvalues. We then used the subroutines DGECO and DGESL from the LINPACK package [27] to solve the linear system obtained when Eq. (63) was substituted into Eq. (25) evaluated at the quadrature points, and so the solution was established.

Finally, but importantly, we note that since the function $\Psi(\xi)$ given by Eq. (23) can, for case 1 and case 3, be zero from a computational point-of-view, we can have some, say a total of N_0, of the quadrature points $\{\xi_i\}$ equal to some of the separation constants

Table 1. *The viscous-slip coefficient* ζ

model	$\alpha = 0.1$	$\alpha = 0.3$	$\alpha = 0.5$	$\alpha = 0.7$	$\alpha = 0.9$	$\alpha = 1$
case 1	17.10313	5.255112	2.861190	1.818667	1.227198	1.016191
case 2	17.00079	5.165447	2.783682	1.752827	1.172569	9.670050(−1)
case 3	17.01536	5.178235	2.794754	1.762247	1.180396	9.740570(−1)

Table 2. *The velocity defect* $q_d = x + \zeta - q(x)$

		$\alpha = 0.1$			$\alpha = 0.9$	
x	case 1	case 2	case 3	case 1	case 2	case 3
0.0	6.420697(−1)	4.570891(−1)	5.015427(−1)	3.432612(−1)	2.481908(−1)	2.716527(−1)
0.1	4.678216(−1)	3.166831(−1)	3.511255(−1)	2.531399(−1)	1.736520(−1)	1.921280(−1)
0.2	3.849266(−1)	2.513896(−1)	2.807790(−1)	2.092257(−1)	1.383361(−1)	1.542030(−1)
0.3	3.274692(−1)	2.071135(−1)	2.328409(−1)	1.785271(−1)	1.142336(−1)	1.281834(−1)
0.4	2.838608(−1)	1.742227(−1)	1.970619(−1)	1.551002(−1)	9.625610(−2)	1.086802(−1)
0.5	2.491653(−1)	1.486025(−1)	1.690639(−1)	1.363869(−1)	8.221152(−2)	9.337100(−2)
0.6	2.207284(−1)	1.280398(−1)	1.464913(−1)	1.210013(−1)	7.091383(−2)	8.099879(−2)
0.7	1.969331(−1)	1.111883(−1)	1.279102(−1)	1.080943(−1)	6.163824(−2)	7.079455(−2)
0.8	1.767122(−1)	9.716229(−2)	1.123762(−1)	9.710268(−2)	5.390614(−2)	6.224991(−2)
0.9	1.593216(−1)	8.534641(−2)	9.923244(−2)	8.763227(−2)	4.738402(−2)	5.501011(−2)
1.0	1.442204(−1)	7.529561(−2)	8.800326(−2)	7.939544(−2)	4.182999(−2)	4.881753(−2)
1.4	9.984283(−2)	4.714830(−2)	5.623679(−2)	5.511766(−2)	2.624398(−2)	3.126069(−2)
1.8	7.158058(−2)	3.064916(−2)	3.728946(−2)	3.959614(−2)	1.708383(−2)	2.075917(−2)
2.0	6.118756(−2)	2.496093(−2)	3.066825(−2)	3.387546(−2)	1.392103(−2)	1.708343(−2)
2.5	4.221371(−2)	1.527173(−2)	1.922621(−2)	2.341170(−2)	8.526978(−3)	1.072298(−2)
3.0	2.981274(−2)	9.571427(−3)	1.234550(−2)	1.655706(−2)	5.348931(−3)	6.892023(−3)
5.0	8.597390(−3)	1.711436(−3)	2.432912(−3)	4.792270(−3)	9.585329(−4)	1.361492(−3)

$\{v_j\}$. Of course this is not allowed in our solution, and so, since the quadrature points where $\Psi(\xi_i)$ is effectively zero make no contribution to the right-hand side of Eq. (45), we have simply omitted these quadrature points (and the offending separation constants) from our calculation. In omitting these N_0 quadrature points we have effectively changed N to $N - N_0$ in some aspects of our final calculation.

To complete our work we list in Tables 1 and 2 some results obtained from our FORTRAN implementation of the developed solution of the Kramers problem for the three explicitly considered cases. We note that our results are given with what we believe to be seven figures of accuracy. While we have no proof of the accuracy achieved in this work, we have done some things to support the confidence we have. First of all our results for case 1 agree perfectly with some calculations done previously in a work [28] devoted exclusively to the classical BGK model. Secondly we used the MAPLE V software to evaluate Williams' exact result [3] (for case 2 with $\alpha = 1$ and in our notation)

$$\zeta = \frac{15}{16}\pi^{-1/2} \int_0^\infty \left[\frac{\frac{4}{3}t^3 + 5t - (5 + 3t^2)\arctan t}{\frac{2}{3}t^3 + t - (1 + t^2)\arctan t} \right] \frac{\mathrm{d}t}{t^2} \tag{68}$$

to obtain $\zeta = 0.9670050$ which agrees perfectly with our result. In regard to case 3, we found good agreement (once consistent choices of the scale factors were used) with the calculations of Loyalka [8] and Loyalka & Hickey [9] for the slip coefficient and for the velocity defect for the case without specular reflection. We note also that Loyalka [29] has reported finding good agreement, for all three models considered in this work, with our results for the slip coefficient and the velocity defect relevant to the cases of specular reflection listed in our tables. After some rescaling, we have also confirmed the values of the slip coefficient for cases 1 and 2, with $\alpha = 1$, reported by Cercignani, Foresti & Sernagiotto [30]. Finally we have increased the value of N is our calculation until we found stability in the results.

We note that we have typically used $N = 100$ to generate the results listed in our tables and that the computational time required for our FORTRAN implementation of the solution (with $N = 100$), for all three cases considered at the same time, is less than a second on a 400 MHz Pentium-based PC. Finally, to have some idea about N_0, the number of quadrature points not included in some parts of our calculation, we note that using $\epsilon = 10^{-14}$ to decide if an eigenvalue and a quadrature point were the same 'computationally' and $N = 100$, we found $N_0 = 3$, $N_0 = 0$ and $N_0 = 8$ respectively for the three cases.

6 Final comments

It is clear that the formalism reported here can readily be used to solve other classical problems, in semi-infinite media and for plane-parallel channel flow, in rarefied-gas dynamics when a variant of the CLF model equation is required to give (perhaps) more realistic results than the standard BGK model can provide. In this regard it is worthwhile to note from our tables that the Williams model and the BGK model appear to provide upper and lower bounds for the rigid-sphere model. This observation (should it be proved to be true) could be useful since the calculations for case 1 and case 2 are simpler to implement numerically than for case 3. Finally we note that Loyalka & Hickey [9] have reported numerical results based on an extended (to two terms) version of the one-term CLF equation, and so this more general model equation would appear to be a good candidate for additional work with the discrete-ordinates method discussed herein.

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References

[1] Cercignani, C. (1969) *Mathematical Methods in Kinetic Theory*, Plenum Press, New York.
[2] Cercignani, C. (1988) *The Boltzmann Equation and its Applications*, Springer-Verlag, New York.
[3] Williams, M. M. R. (1971) *Mathematical Methods in Particle Transport Theory*, Butterworth, London.

[4] Bhatnagar, P. L., Gross, E. P. & Krook, M. (1954) A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems, *Phys. Rev.* **94**, 511.

[5] Williams, M. M. R. (1969) Boundary-value problems in the kinetic theory of gases Part I. Slip flow, *J. Fluid Mechs.* **36**, 145.

[6] Cercignani, C. (1966) The method of elementary solutions for kinetic models with velocity-dependent collision frequency, *Ann. Phys. (NY)*, **40**, 469.

[7] Loyalka, S. K. & Ferziger, J. H. (1967) Model dependence of the slip coefficient, *Phys. Fluids* **10**, 1833.

[8] Loyalka, S. K. (1975) Velocity profile in the Knudsen layer for Kramer's problem, *Phys. Fluids* **18**, 1666.

[9] Loyalka, S. K. & Hickey, K. A. (1989) Velocity slip and defect: Hard sphere gas, *Phys. Fluids A* **1**, 612.

[10] Loyalka, S. K. & Hickey, K. A. (1990) The Kramers problem: Velocity slip and defect for a hard sphere gas with arbitrary accommodation, *Z. Angew. Math. Phys.* **41**, 245.

[11] Busbridge, I. W. (1953) Coherent and non-coherent scattering in the theory of line formation, *Monthly Notices Royal Astronomical Society*, **113**, 52.

[12] Bednarz, R. J. & Mika, J. (1963) Energy-dependent Boltzmann equation in plane geometry, *J. Math. Phys.* **4**, 1285.

[13] Barichello, L. B. & Siewert, C. E. (1999) A discrete-ordinates solution for a non-grey model with complete frequency redistribution, *J. Quant. Spectros. Radiat. Transfer* **62**, 665.

[14] Chandrasekhar, S. (1950) *Radiative Transfer*, Oxford University Press, London.

[15] Williams, M. M. R., A review of the rarefied gas dynamics theory associated with some classical problems in flow and heat transfer, *Z. Angew. Math. Phys.* in press.

[16] Barichello, L. B. & Siewert, C. E. (1998) On the equivalence between the discrete-ordinates and the spherical-harmonics methods in radiative transfer, *Nucl. Sci. Eng.* **130**, 79.

[17] Siewert, C. E. (2000) A concise and accurate solution to Chandrasekhar's basic problem in radiative transfer, *J. Quant. Spectros. Radiat. Transfer* **64**, 109.

[18] Siewert, C. E. (2000) A discrete-ordinates solution for radiative-transfer models that include polarization effects, *J. Quant. Spectros. Radiat. Transfer* **64**, 227.

[19] Barichello, L. B. & Siewert, C. E. (1999) A discrete-ordinates solution for a polarization model with complete frequency redistribution, *The Astrophys. J.* **513**, 370.

[20] Barichello, L. B. & Siewert, C. E. (2000) The searchlight problem for radiative transfer in a finite slab, *J. Comp. Phys.* **157**, 707.

[21] Barichello, L. B., Rodrigues, P. & Siewert, C. E., A discrete-ordinates solution for dual-mode heat transfer in a cylinder, submitted for publication.

[22] Sharipov, F. & Seleznev, V. (1998) Data on internal rarefied gas flows, *J. Phys. Chem. Ref. Data* **27**, 657.

[23] Arkeryd, L. & Illner, R. (1995) The Broadwell model in a box: strong L^1-convergence to equilibrium, *SIAM J. Applied Math.* **55**, 641.

[24] Broadwell, J. E. (1964) Shock structure in a simple discrete velocity gas, *Phys. Fluids* **7**, 1243.

[25] Datta, B. N. (1995) *Numerical Linear Algebra and Applications*, Brooks/Cole, Pacific Grove.

[26] Siewert, C. E. & Wright, S. J. (1999) Efficient eigenvalue calculations in radiative transfer, *J. Quant. Spectrosc. Radiat. Transfer* **62**, 685.

[27] Dongarra, J. J., Bunch, J. R., Moler, C. B. & Stewart, G. W. (1979) *LINPACK User's Guide*, SIAM, Philadelphia.

[28] Barichello, L. B., Camargo, M., Rodrigues, P. & Siewert, C. E., Unified solutions to classical flow problems based on the BGK model, *Z. Angew. Math. Phys.* in press.

[29] Loyalka, S. K. (2000) personal communication.

[30] Cercignani, C., Foresti, P. & Sernagiotto, F. (1968) Dependence of the slip coefficient on the form of the collision frequency, *Il Nuovo Cimento* **LVII B**, 297.