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On computing the Chapman-Enskog and Burnett functions

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Abstract

An expansion and projection technique based on Legendre polynomials is used to solve, in an efficient and accurate way, the Chapman-Enskog equations for viscosity and heat transfer and to compute the Burnett functions required, for example, for Poiseuille-flow problems based on rigid-sphere collisions and the linearized Boltzmann equation.

Keywords: Boltzmann equation; Rarefied-gas dynamics; Chapman-Enskog; Burnett

1. Introduction

Within the context of the linearized Boltzmann equation for rigid-sphere collisions, the Chapman-Enskog functions for viscosity and heat transfer, as well as the Burnett functions, have been computed and the results reported [1–4]. However, since these functions are especially important in regard to analytical and computational solutions of the linearized Boltzmann equation, we report here an additional calculation that can be used as an alternative to the previously reported [1,4] computations that were based on the use of spline functions. While we consider the algorithm, based on Hermite cubic splines and a collocation procedure, that was used in Ref. [4] to be a good one, we wish here to report a computation that leads to the same numerical results, without any of the concerns that collocation methods can sometimes provoke. Since much of the introductory material we require in this work can be found in Ref. [4], we can be brief here.

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The general class of problems we consider can be written as

$$\mathscr{L}_n\{f\}(c) = r(c), \quad c \in [0,\infty), \tag{1}$$

with $r(c)$ given, and with

$$\mathscr{L}_n\{f\}(c) = \nu(c) f(c) - \int_0^\infty \mathrm{e}^{-c'^2} f(c') k_n(c', c) c'^2 \, \mathrm{d}c'. \tag{2}$$

Here

$$\nu(c) = \frac{2c^2+1}{c} \int_0^c \mathrm{e}^{-x^2} \, \mathrm{d}x + \mathrm{e}^{-c^2} \tag{3}$$

is the "collision frequency" and the functions $k_n(c', c)$ are components in the Pekeris-Alterman "rigid-sphere" scattering kernel [2] written as

$$K(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi} \sum_{n=0}^{\infty} \sum_{m=0}^{n} (2n+1)(2-\delta_{0,m}) P_n^m(\mu') P_n^m(\mu) k_n(c', c) \cos m(\chi' - \chi). \tag{4}$$

The *normalized* Legendre functions

$$P_n^m(\mu) = \left[\frac{(n-m)!}{(n+m)!}\right]^{1/2} (1-\mu^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}\mu^m} P_n(\mu), \quad n \geqslant m, \tag{5}$$

where $P_n(\mu)$ denotes the usual Legendre polynomial, are such that

$$\int_{-1}^{1} P_n^m(\mu) P_{n'}^m(\mu) \, \mathrm{d}\mu = \left(\frac{2}{2n+1}\right) \delta_{n,n'}. \tag{6}$$

In this work we use the component functions $k_n(c', c)$ only for $n = 0, 1, 2$ and 3. Since these basic functions were listed explicitly in Ref. [4], we feel no need to re-list them here.

We note [5] that as a result of the fact that the collisional invariants (corresponding to conservation of mass, energy and momentum) are solutions of the homogeneous linearized Boltzmann equation, there are three basic identities, viz.

$$\nu(c) = \int_0^\infty \mathrm{e}^{-c'^2} k_0(c', c) c'^2 \, \mathrm{d}c', \tag{7a}$$

$$\nu(c) c = \int_0^\infty \mathrm{e}^{-c'^2} k_1(c', c) c'^3 \, \mathrm{d}c' \tag{7b}$$

and

$$\nu(c) c^2 = \int_0^\infty \mathrm{e}^{-c'^2} k_0(c', c) c'^4 \, \mathrm{d}c' \tag{7c}$$

that are relevant to Eq. (1). Since Eqs. (7) show that the homogeneous versions of Eq. (1) have solutions for $n = 0$ and 1, we can list solvabilitly conditions

$$\int_0^\infty \mathrm{e}^{-c^2} \begin{bmatrix} 1 \\ c^2 \end{bmatrix} r(c) c^2 \, \mathrm{d}c = \mathbf{0}, \quad n = 0, \tag{8a}$$

and

$$\int_0^\infty \mathrm{e}^{-c^2} r(c) c^3 \, \mathrm{d}c = 0, \quad n = 1, \tag{8b}$$

that must be satisfied for these two cases. While the numerical approach we use is general, the specific cases considered here are the Chapman-Enskog equation for viscosity,

$$\mathscr{L}_2\{B\}(c) = c^2, \tag{9}$$

the Chapman-Enskog equation for heat transfer,

$$\mathscr{L}_1\{A\}(c) = c(c^2 - 5/2), \tag{10a}$$

with the normalization condition

$$\int_0^\infty \mathrm{e}^{-c^2} A(c) c^3 \, \mathrm{d}c = 0, \tag{10b}$$

and the two Burnett equations [1]

$$\mathscr{L}_1\{D\}(c) = 2cB(c) - 5c\varepsilon_\mathrm{p}, \tag{11a}$$

with the normalization [1]

$$\int_0^\infty \mathrm{e}^{-c^2} D(c) c^3 \, \mathrm{d}c = 0, \tag{11b}$$

and

$$\mathscr{L}_3\{E\}(c) = 2cB(c). \tag{12}$$

Here

$$\varepsilon_\mathrm{p} = \frac{16}{15}\pi^{-1/2} \int_0^\infty \mathrm{e}^{-c^2} B(c) c^4 \, \mathrm{d}c. \tag{13}$$

We note that while not referred to as Burnett equations, terminology taken from Ref. [1], Eqs. (11) and (12) have also been discussed, for example, by Simons [6] and Williams [7].

2. The algorithm

We start by expressing the desired (approximate) solution of Eq. (1) as

$$f(c) = \sum_{k=0}^{K} a_k P_k(2\mathrm{e}^{-c} - 1) \tag{14}$$

where the constant $\{a_k\}$ are to be determined. To keep our notation simple, we (sometimes) omit the subscript n used in Eqs. (1) and (2) to denote a specific kernel function $k_n(c', c)$. We note that an expansion of the form of Eq. (14) was used in Refs. [8] and [9] to solve many of the classical problems in rarefied gas dynamics based on the linearized Boltzmann equation and the rigid-sphere interaction law. However, in Refs. [8] and [9] the quantities of interest were expressed in terms of moments (integrals over the velocity) of the particle velocity distribution function, while here we

seek to compute the function $f(c)$ itself. To find the coefficients $\{a_k\}$ required in Eq. (14), we substitute Eq. (14) into Eq. (1), multiply the resulting equation by

$$\boldsymbol{W}(c) = \boldsymbol{P}^{\mathrm{T}}(c)c^2\mathrm{e}^{-c^2}, \tag{15}$$

where

$$\boldsymbol{P}(c) = [P_0(2\mathrm{e}^{-c} - 1), P_1(2\mathrm{e}^{-c} - 1), \ldots, P_K(2\mathrm{e}^{-c} - 1)], \tag{16}$$

and integrate over all c to obtain the system of linear algebraic equations

$$(\boldsymbol{S} - \boldsymbol{B}_n)\boldsymbol{A} = \boldsymbol{R}. \tag{17}$$

Here we use the superscript T to denote the transpose operation, the vector $\boldsymbol{A}$ contains the desired constants $\{a_k\}$,

$$\boldsymbol{S} = \int_0^\infty \mathrm{e}^{-c^2}\boldsymbol{P}^{\mathrm{T}}(c)\boldsymbol{P}(c)v(c)c^2\,\mathrm{d}c, \tag{18}$$

$$\boldsymbol{R} = \int_0^\infty \mathrm{e}^{-c^2}\boldsymbol{P}^{\mathrm{T}}(c)r(c)c^2\,\mathrm{d}c \tag{19}$$

and

$$\boldsymbol{B}_n = \int_0^\infty \int_0^\infty \mathrm{e}^{-c^2}\mathrm{e}^{-c'^2}\boldsymbol{P}^{\mathrm{T}}(c)\boldsymbol{P}(c')k_n(c', c)c^2c'^2\,\mathrm{d}c'\,\mathrm{d}c. \tag{20}$$

Since the kernel functions are such that $k_n(c', c)=k_n(c, c')$, we see that the matrices $\boldsymbol{B}_n$ are symmetric (a fact that can be used to reduce the numerical work required to evaluate these matrices). However, as mentioned in Refs. [8] and [9], some care must be exercised in evaluating the kernel functions $k_n(c', c)$.

After we solve the linear system given as Eq. (17) our first solution is given by Eq. (14); however an alternative "post-processed" result can be obtained by using Eq. (14) in Eq. (1) to find

$$f(c) = \left[r(c) + \sum_{k=0}^{K} a_k F_k(c)\right] \Big/ v(c) \tag{21}$$

where

$$F_k(c) = \int_0^\infty \mathrm{e}^{-c'^2}P_k(2\mathrm{e}^{-c'} - 1)k_n(c', c)c'^2\,\mathrm{d}c'. \tag{22}$$

Our results for the functions $B(c)$ and $E(c)$ are given by either Eq. (14) or Eq. (21); however, since Eq. (7b) shows that a function $h(c) = c$ is a solution of the homogeneous versions of Eqs. (10a) and (11a), we can write

$$A(c) = A_0(c) - \beta c \tag{23}$$

and

$$D(c) = D_0(c) - \gamma c \tag{24}$$

where $A_0(c)$ and $D_0(c)$ are given by either of Eqs. (14) and (21). It follows that we can use the normalization conditions listed as Eqs. (10b) and (11b) to define the constants β and γ. And so we substitute Eq. (23) into Eq. (10b) and Eq. (24) into Eq. (11b) to find

$$\beta = \frac{8}{3\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} A_0(c) c^3 \, \mathrm{d}c \tag{25}$$

and

$$\gamma = \frac{8}{3\pi^{1/2}} \int_0^\infty \mathrm{e}^{-c^2} D_0(c) c^3 \, \mathrm{d}c. \tag{26}$$

To be clear, we note again that while either of Eqs. (14) and (21) can be used to define $A_0(c)$ and $D_0(c)$, our final results for $A(c)$ and $D(c)$ are given by Eqs. (23) and (24) with the constants β and γ given by Eqs. (25) and (26).

3. Numerical results

In evaluating our numerical solutions for the two Chapman-Enskog functions $A(c)$ and $B(c)$ and the two Burnett functions $D(c)$ and $E(c)$, we consider, as have others [1–4], that the domain of significant interest is the subset $c \in [0, 5]$ of the complete domain $[0, \infty)$. As the use of these functions typically involves a multiplication by $\exp(-c^2)$ the chosen domain of interest seems suitable for various applications that require these functions. Since the numerical results we obtained here are essentially in perfect agreement with our previous work, we need not list these results again. However, some general comments on the implementation of the developed algorithms can be given. In our work here we have two basic approximation parameters: $K + 1$ is the number of basis functions used in Eq. (14) and M is the number of Gauss points used to evaluate the input matrices defined by Eqs. (18)–(20) and (22). While we have not attempted a definitive study to find the minimum values of K and M to obtain a given degree of accuracy, we did find that we could recover the seven-digit results listed in Ref. [4] with $K = 100$ and $M = 200$. More importantly we found, for $c \in [0, 5]$, that we had to use the post-processed result listed as Eq. (21) only for, say, $c < 0.2$ and $c > 4.2$. And so, since we found the desired results mostly from the simple result listed as Eq. (14), our final algorithm was especially efficient.

Since we intend to use these basic Chapman-Enskog and Burnett functions in conjunction with general computations in rarefied gas dynamics, our goal here was to produce (FORTRAN) subroutines that would yield these functions quickly and accurately. In order not to have to compute the input matrices more that once, we simply "hard-wired" the constants $\{a_k\}$, for each of the four functions, into our subroutines. In this way, we were able to reproduce the table of results listed with seven digits of accuracy in Ref. [4] in less than 0.2s on a 1.2 Ghz mobile Pentium III processor. And so we conclude that the algorithms developed here provide a very convenient alternative to those based on Hermite cubic splines and collocation [1,4].

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References

[1] Loyalka SK, Hickey KA. Plane Poiseuille flow: near continuum results for a rigid sphere gas. Physica A 1989;160: 395–408.
[2] Pekeris CL, Alterman Z. Solution of the Boltzmann-Hilbert integral equation II. The coefficients of viscosity and heat conduction. Proc Natl Acad Sci 1957;43:998–1007.
[3] Ohwada T, Sone Y. Analysis of thermal stress slip flow and negative thermophoresis using the Boltzmann equation for hard-sphere molecules. Eur J Mech B/Fluids 1992;11:389–414.
[4] Siewert CE. On computing the Chapman-Enskog functions for viscosity and heat transfer and the Burnett functions. JQSRT 2002;74:789–96.
[5] Barichello LB, Siewert CE. Some comments on modeling the linearized Boltzmann equation. JQSRT 2003;77:43–59.
[6] Simons S. Poiseuille gas flow in the transition regime I. Formulation of the general theory. Proc Roy Soc A 1967;301:387–400.
[7] Williams MMR. Mathematical methods in particle transport theory. London: Butterworth, 1971.
[8] Siewert CE. The linearized Boltzmann equation: a concise and accurate solution of the temperature-jump problem. JQSRT 2003;77:417–32.
[9] Siewert CE. The linearized Boltzmann equation: concise and accurate solutions to basic flow problems. Z Angew Math Phys 2003;54:273–303.