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Note

On computing the Chapman–Enskog functions for viscosity and heat transfer and the Burnett functions

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Abstract

Hermite cubic splines and collocation are 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 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 [1–3]. However, we feel these basic functions are sufficiently important that we can justify reporting an additional calculation and giving enough details of the computation that the algorithms can be readily used by interested readers.

The general class of problems considered here 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

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

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

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

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 only some of the $k_n(c',c)$, and so noting that, in general, $k_n(c',c) = k_n(c,c')$, we make two corrections to the listing in Ref. [1] and write for, $c' < c$,

$$-(1/2)c'ck_0(c',c) = (2/3)c'^3 + 2c'c^2 - 4P(c'), \tag{7a}$$

$$-(1/2)c'^2c^2k_1(c',c) = (2/15)c'^5 - 4c' - (2/3)c'^3c^2 - 4(c'^2-1)P(c'), \tag{7b}$$

$$-(1/2)c'^3c^3k_2(c',c) = a_2(c',c) + b_2(c',c)P(c') \tag{7c}$$

and

$$-(1/2)c'^4c^4k_3(c',c) = a_3(c',c) + b_3(c',c)P(c'), \tag{7d}$$

where

$$a_2(c',c) = (2/35)c'^7 - 3c'^3 + 18c' - [(2/15)c'^5 - 3c']c^2, \tag{8a}$$

$$b_2(c',c) = -6c'^4 + 15c'^2 - 18 + [2c'^2 - 3]c^2, \tag{8b}$$

$$a_3(c',c) = (2/63)c'^9 - 5c'^5 + 20c'^3 - 150c' - [(2/35)c'^7 - c'^3 + 30c']c^2 \tag{8c}$$

and

$$b_3(c',c) = -10c'^6 + 45c'^4 - 120c'^2 + 150 + [6c'^4 - 21c'^2 + 30]c^2. \tag{8d}$$

In addition

$$P(c) = \mathrm{e}^{c^2}\int_0^c \mathrm{e}^{-x^2}\,\mathrm{d}x. \tag{9}$$

We note [4] 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.

$$v(c) = \int_0^\infty \mathrm{e}^{-c'^2} k_0(c', c) c'^2 \, \mathrm{d}c', \tag{10a}$$

$$v(c)c = \int_0^\infty \mathrm{e}^{-c'^2} k_1(c', c) c'^3 \, \mathrm{d}c' \tag{10b}$$

and

$$v(c)c^2 = \int_0^\infty \mathrm{e}^{-c'^2} k_0(c', c) c'^4 \, \mathrm{d}c' \tag{10c}$$

that are relevant to Eq. (1) for the cases $n = 0$ and 1. Since Eqs. (10) show that the homogeneous versions of Eq. (1) have solutions for $n = 0$ and 1, we can list solvability conditions (consequences of a manifestation of the Fredholm Alternative)

$$\int_0^\infty \mathrm{e}^{-c^2} \begin{bmatrix} 1 \\ c^2 \end{bmatrix} r(c) c^2 \, \mathrm{d}c = 0, \quad n = \mathbf{0} \tag{11a}$$

and

$$\int_0^\infty \mathrm{e}^{-c^2} r(c) c^3 \, \mathrm{d}c = 0, \quad n = 1, \tag{11b}$$

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

$$\mathscr{L}_2\{c^2 b\}(c) = c^2, \tag{12}$$

the Chapman–Enskog equation for heat transfer

$$\mathscr{L}_1\{ca\}(c) = c(c^2 - 5/2), \tag{13a}$$

with the normalization condition

$$\int_0^\infty \mathrm{e}^{-c^2} a(c) c^4 \, \mathrm{d}c = 0, \tag{13b}$$

and the two Burnett equations [1]

$$\mathscr{L}_1\{c^3 d\}(c) = 2c^3 b(c) - 5c\varepsilon_\mathrm{p}, \tag{14a}$$

with

$$\varepsilon_\mathrm{p} = \frac{16}{15}\pi^{-1/2} \int_0^\infty \mathrm{e}^{-c^2} b(c) c^6 \, \mathrm{d}c \tag{14b}$$

and the normalization [1]

$$\int_0^\infty \mathrm{e}^{-c^2} d(c) c^6 \, \mathrm{d}c = 0, \tag{14c}$$

and

$$\mathscr{L}_3\{c^3 e\}(c) = 2c^3 b(c). \tag{15}$$

We note that while not referred to as Burnett equations, terminology taken from Ref. [1], Eqs. (14) and (15) have also been discussed, for example, by Simons [5] and Williams [6].

Since we wish to have this work to be self-contained, to have our calculation clearly defined and to introduce some notation, we comment briefly on the spline functions we use.

2. The spline functions

The Hermite cubic spline functions we use in this work are taken from Schultz [7]. To be specific and to define the notation we use, we list these splines here. First of all, we consider there to be $M+1$ knots ζ_α defined on the interval [0,1] by

$$\zeta_\alpha = (\alpha/M)^m, \quad \alpha = 0, 1, \ldots, M. \tag{16}$$

In this work we use the quadratic distribution ($m = 2$). And so to approximate a function, say $Y(x)$, for $x \in [0, 1]$, in terms of the spline functions we write

$$Y(x) = \sum_{\alpha=0}^{K} a_\alpha \mathscr{F}_\alpha(x), \tag{17}$$

where the a_α are constants and where $K = 2M + 1$. We note that there are two spline functions $\mathscr{F}_\alpha(x)$ associated with each knot and that the spline functions are defined differently for even or odd values of α. And so we write

$$\mathscr{F}_{2\beta}(x) = \Phi_\beta(x) \quad \text{and} \quad \mathscr{F}_{2\beta+1}(x) = \Psi_\beta(x) \tag{18a,b}$$

for $\beta = 0, 1, \ldots, M$. Making use of the definitions

$$p_\alpha(x) = \frac{x - \zeta_{\alpha-1}}{\zeta_\alpha - \zeta_{\alpha-1}} \tag{19a}$$

and

$$g_\alpha(x) = \frac{\zeta_{\alpha+1} - x}{\zeta_{\alpha+1} - \zeta_\alpha} \tag{19b}$$

and considering that the spline functions are zero unless otherwise defined, we can write the Φ functions as

$$\Phi_0(x) = g_0^2(x)[3 - 2g_0(x)], \quad x \in [\zeta_0, \zeta_1], \tag{20a}$$

$$\Phi_\alpha(x) = \begin{cases} p_\alpha^2(x)[3 - 2p_\alpha(x)], & x \in [\zeta_{\alpha-1}, \zeta_\alpha], \\ g_\alpha^2(x)[3 - 2g_\alpha(x)], & x \in [\zeta_\alpha, \zeta_{\alpha+1}], \end{cases} \tag{20b}$$

for $\alpha = 1, 2, \ldots, M-1$, and

$$\Phi_M(x) = p_M^2(x)[3 - 2p_M(x)], \quad x \in [\zeta_{M-1}, \zeta_M]. \tag{20c}$$

In a similar way we can write the Ψ functions as

$$\Psi_0(x) = x g_0^2(x), \quad x \in [\zeta_0, \zeta_1], \tag{21a}$$

$$\Psi_\alpha(x) = \begin{cases} (x - \zeta_\alpha) p_\alpha^2(x), & x \in [\zeta_{\alpha-1}, \zeta_\alpha], \\ (x - \zeta_\alpha) g_\alpha^2(x), & x \in [\zeta_\alpha, \zeta_{\alpha+1}], \end{cases} \tag{21b}$$

for $\alpha = 1, 2, \ldots, M-1$, and

$$\Psi_M(x) = (x - \zeta_M) p_M^2(x), \quad x \in [\zeta_{M-1}, \zeta_M]. \tag{21c}$$

Having defined the spline functions we use, we are ready to proceed with our calculations.

3. The algorithm

Before beginning this computation, a remark or two could be helpful. While the component kernel functions defined by Eqs. (7)–(9) are continuous, the derivative of these functions has a discontinuity at $c=c'$. And it is (mainly) for this reason why a standard quadrature scheme defined over the entire interval $[0,\infty)$ cannot be expected to integrate well these functions. Of course, to split the integration interval at $c'=c$ is clearly the right approach, but this approach results in integrals with variable limits which introduce new challenges within the context, say, of a discrete-ordinates approximation. The use of the spline functions, on the other hand, is convenient here. To make use of the interval $[0,1]$, we introduce the variables

$$u(c)=\mathrm{e}^{-c} \quad \text{and} \quad u'(c')=\mathrm{e}^{-c'} \tag{22a,b}$$

and rewrite our problem as

$$v(-\ln u)f(-\ln u)-\int_0^1 f(-\ln u')k(-\ln u',-\ln u)J(u')\,\mathrm{d}u'=r(-\ln u) \tag{23}$$

for $u\in[0,1]$. Here, to keep the notation simple, we have omitted the subscript n that labels the functions $k(c',c)$, and we let

$$J(u)=(1/u)(\ln u)^2\mathrm{e}^{-(\ln u)^2}. \tag{24}$$

We now introduce the spline representation

$$f(-\ln u)=\sum_{\alpha=0}^{K} a_\alpha \mathscr{F}_\alpha(u) \tag{25}$$

into Eq. (23) to obtain

$$\sum_{\alpha=0}^{K} a_\alpha[v(-\ln u)\mathscr{F}_\alpha(u)-U_\alpha(u)-V_\alpha(u)]=r(-\ln u), \tag{26}$$

where

$$U_\alpha(u)=\int_0^u \mathscr{F}_\alpha(u')k(-\ln u',-\ln u)J(u')\,\mathrm{d}u' \tag{27a}$$

and

$$V_\alpha(u)=\int_u^1 \mathscr{F}_\alpha(u')k(-\ln u',-\ln u)J(u')\,\mathrm{d}u'. \tag{27b}$$

The approach we use here is based on collocation. We thus evaluate Eq. (26) at the collocation points

$$u_\alpha=(\alpha/K)^m, \quad \alpha=0,1,\ldots,K, \tag{28}$$

(again with $m=2$) and solve the resulting system of linear algebraic equations to find the coefficients $\{a_\alpha\}$. Finally, rather than using Eq. (25), we substitute that result into the integral term of Eq. (23) to obtain the "post-processed" result

$$f(c)=\left\{r(c)+\sum_{\alpha=0}^{K} a_\alpha[U_\alpha(\mathrm{e}^{-c})+V_\alpha(\mathrm{e}^{-c})]\right\}\Big/v(c) \tag{29}$$

that is valid for all c. Having defined the basics of our computation, we comment on the important issue of how we evaluate the U and V functions. Considering that $[\alpha_k, \beta_k]$ is the support of the spline function $\mathscr{F}_k(x)$, i.e.

$$\mathscr{F}_k(x) = 0, \quad x \notin [\alpha_k, \beta_k], \tag{30}$$

we can write

$$U_k(u) = 0, \quad u \leqslant \alpha_k, \tag{31a}$$

and

$$U_k(u) = \int_{\alpha_k}^{\min\{u,\beta_k\}} \mathscr{F}_\alpha(u')k(-\ln u', -\ln u)J(u')\,\mathrm{d}u', \quad x > \alpha_k. \tag{31b}$$

In a similar way we can write

$$V_k(u) = 0, \quad u \geqslant \beta_k, \tag{32a}$$

and

$$V_k(u) = \int_{\max\{u,\alpha_k\}}^{\beta_k} \mathscr{F}_\alpha(-\ln u')k(-\ln u', -\ln u)J(u')\,\mathrm{d}u', \quad u < \beta_k. \tag{32b}$$

Now since the spline functions have different definitions on each of two subintervals of $[\alpha_k, \beta_k]$, we use a Gauss–Legendre scheme over each one of these subintervals to evaluate the required integrals. In this way, we can obtain good accuracy for the integrals with a very low-order quadrature scheme. In fact, to evaluate the U and V functions well with a low-order quadrature scheme is what makes this computation especially efficient as well as accurate.

4. Numerical results

As our first calculation we consider the Chapman–Enskog viscosity problem. We note that we have only two parameters in our computation: the number of knots $M + 1$ and the order N of the Gauss–Legendre quadrature scheme used to evaluate the U and V functions. While we have made no definitive study of minimum values for M and N required for a given degree of accuracy, we did find that we could reproduce the results given in Refs. [1–3] with $M = 300$ and $N = 4$. Our FORTRAN implementation with these parameters runs in 15 s on a 400 MHz Pentium-based PC. Having made a FORTRAN subroutine to define $c^2 b(c)$ with these parameters, we used 100 Gauss–Legendre points and the map given by Eq. (22a) to find (in less than 2 s) from

$$\varepsilon_\mathrm{p} = \frac{16}{15}\,\pi^{-1/2} \int_0^\infty \mathrm{e}^{-c^2} b(c) c^6\,\mathrm{d}c \tag{33}$$

the result

$$\varepsilon_\mathrm{p} = 0.449027806\ldots. \tag{34}$$

Table 1
The basic functions

c	$ca(c)$	$c^2b(c)$	$c^3d(c)$	$c^3e(c)$
0.0	0.0	0.0	0.0	0.0
0.1	−2.157649(−1)	6.195829(−3)	−1.843725(−1)	6.343351(−4)
0.2	−4.242989(−1)	2.466807(−2)	−3.611823(−1)	5.016259(−3)
0.3	−6.186095(−1)	5.508042(−2)	−5.232815(−1)	1.661186(−2)
0.4	−7.921517(−1)	9.690213(−2)	−6.642904(−1)	3.837047(−2)
0.5	−9.389864(−1)	1.494472(−1)	−7.788429(−1)	7.256883(−2)
1.0	−1.114455	5.437725(−1)	−8.442335(−1)	4.609468(−1)
1.5	−1.138869(−1)	1.083802	−7.351806(−4)	1.165430
2.0	2.208681	1.696714	1.651005	2.053253
2.5	5.899307	2.342811	3.970062	3.020008
3.0	1.097512(1)	3.002212	6.842049	4.008393
3.5	1.744438(1)	3.665129	1.018088(1)	4.991261
4.0	2.531190(1)	4.326807	1.392144(1)	5.957431
4.5	3.458077(1)	4.985040	1.801342(1)	6.903581
5.0	4.525312(1)	5.638929	2.241714(1)	7.830029

The computation for the Chapman–Enskog equation for heat flow required a modest amount of additional effort since a constant added to the spline solution must be fixed so that the final result satisfies Eq. (13b). Here with the same parameters, we found from

$$\varepsilon_t = \frac{16}{15}\,\pi^{-1/2}\int_0^\infty \mathrm{e}^{-c^2} a(c) c^6\,\mathrm{d}c \tag{35}$$

the result

$$\varepsilon_t = 0.679630049\ldots. \tag{36}$$

While the evaluation of the basic quantities ε_p and ε_t yielded many correct significant figures, we cannot, of course, claim that our functions $c^2b(c)$ and $ca(c)$ are uniformly that good. But, we believe that our algorithm can be used with confidence.

To complete this note, we list in Table 1 some numerical results we found from the algorithms discussed here. Of course these results are not in sufficient quantity that they can be used for practical problems, but they can be useful as test results for a code developer. We note that the results given in three of the four columns of Table 1 are consistent with the results of Loyalka and Hickey [1], but the results listed in the third column [when divided by ε_p] do not agree with the second column of Table 1 in Ref. [1]. We believe the numerical results listed in Ref. [3] can be used to justify the confidence we have that all numerical results reported here can be considered correct (to all given digits).

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