Pseudospectral Methods of Solution of the Linear and Linearized Boltzmann Equations; Transport and Relaxation

Bernie D. Shizgal

Laboratoire Dieudonné, Université de Nice Sophia Antipolis, Nice, France,
and
Department of Chemistry, University of British Columbia, Vancouver, BC V6T1Z1, Canada

Abstract. The study of the solution of the linearized Boltzmann equation has a very long history arising from the classic work by Chapman and Cowling. For small departures from a Maxwellian, the nonlinear Boltzmann equation can be linearized and the transport coefficients calculated with the Chapman-Enskog approach. This procedure leads to a set of linear integral equations which are generally solved with the expansion of the departure from Maxwellian in Sonine polynomials. The method has been used successfully for many decades to compare experimental transport data in atomic gases with theory generally carried out for realistic atom-atom differential cross sections. There are alternate pseudospectral methods which involve the discretization of the distribution function on a discrete grid. This paper considers a pseudospectral method of solution of the linearized hard sphere Boltzmann equation for the viscosity in a simple gas. The relaxation of a small departure from a Maxwellian is also considered for the linear test particle problem with unit mass ratio which is compared with the relaxation for the linearized one component Boltzmann equation.

INTRODUCTION

The Chapman-Enskog approach to the calculation of transport coefficients in a simple gas is very well known and described in standard texts [1]. A small departure from a Maxwellian is assumed to occur owing to small velocity and/or temperature gradients. The transport coefficients are then defined by the linear phenomenological laws. With this approach, the viscosity of a simple gas is given by

$$\varepsilon_p = \frac{16\sqrt{2}}{15} \int_0^\infty e^{-x^2} x^4 B(x) dx, \tag{1}$$

in reduced units as defined elsewhere [2, 3, 4]. The function $B(x)$ is the solution of the linear integral equation

$$\int_0^\infty e^{-x^2} x^2 K_2(x,y) B(x)] dx - Z(y) B(y) = -y^2, \tag{2}$$

where the symmetric kernel, $K_2(x,y)$, for $x < y$ is given by

$$
\begin{aligned}
K_2(x,y) &= -2[A(x,y) + C(x,y)\Psi(x)]/(x^4 y^4), \\
A(x,y) &= \frac{2}{35}x^7 - 3x^3 + 18x - y^2(\frac{2}{15}x^5 - 3x), \\
C(x,y) &= -6x^4 + 15x^2 - 18 + y^2(2x^2 - 3)
\end{aligned}
\tag{3}
$$

and $\Psi(x) = \sqrt{\pi} e^{x^2} \mathrm{erf}(x)/2$ and $\mathrm{erf}(x)$ is the error function. The kernel $K_2(x,y)$ is the $\ell = 2$ component of the expansion of the anisotropic kernel in Legendre polynomials, that is, $K(x,y,\mu) = \sum_\ell K_\ell(x,y) P_\ell(\mu)$ and μ is the cosine of the angle between the velocities **x** and **y** [2, 3, 4, 5]. It is important to note that function $B(x)$ in this paper corresponds to $x^2 b(x)$ in the papers by Siewert [2] and Loyalka et al [3]. In Eq. (2), $Z(x)$ is the collision frequency defined by

$$Z(x) = \frac{\sqrt{\pi}}{2}(2x + \frac{1}{x})\mathrm{erf}(x) + e^{-x^2}. \tag{4}$$

In recent years, there has been a renewed interest [2, 3, 6] in the solution of the integral equations for the hard sphere potential. The objectives are directed towards the development of accurate and efficient numerical algorithms for the solution of the Boltzmann equation. Loyalka et al [3] have provided extremely accurate solutions (up to 30 significant figures) for the heat conductivity and viscosity coefficients by employing algebraic methods. Their results serve as benchmarks against which other methods can be compared. Siewert [2] used a spline method for the same problem and obtained similar although less accurate results. The importance of these endeavors in rarefied gas dynamics was discussed in [7].

Shizgal [8] introduced a pseudospectral method based on the speed quadrature defined by the Maxwellian weight function, $w(x) = x^2 e^{-x^2}$, which has been used to determine the eigenvalue spectrum of both the linearized operator and the linear operator for binary mixtures [5, 9]. The approach in this paper is based on the observation that the integral for the dimensionless viscosity converges very rapidly with respect to the number, N, of speed quadrature points and weights [8]. With a spline fit of B(x) in Table 5 of [3] which has 44 data for $x \in [0, 6]$, I find that $\varepsilon_p =$ 0.44852, 0.44902, 0.4490280 and 0.4490278 for, N = 2, 4, 6 and 8, respectively. This suggests that a solution based on the speed quadrature points should converge quickly. The integral with the spline parameters with the 44 data points is $\varepsilon_p = 0.4490278$. A Simpson's rule integration with N = 10, 20 and 30, gives $\varepsilon_p = 0.44278$, 0.449032 and 0.4490278, respectively. The relaxation to equilibrium of the one component hard-sphere gaseous system [8, 10] is also studied. This is important in the development of discretization methods for the description of the relaxation to equilibrium for the nonlinear Boltzmann equation [10, 11]. The relaxation behavior for the test particle problem for unit mass ratio with the linear Boltzmann equation is also studied and compared with the results for the one component system.

SOLUTION OF THE BOLTZMANN EQUATION FOR VISCOSITY WITH SPEED QUADRATURE POINTS

The solution of the integral equation, Eq. (2), is often based on the evaluation of the distribution function on a grid of points $\{z_i\}$ defined for a quadrature of the form

$$\int_0^\infty w(x) f(x) dx \approx \sum_{i=1}^N W_i w(z_i) f(z_i), \tag{5}$$

where $\{W_i\}$ are the set of associated weights, $w(x)$ is a weight function and N is the number of quadrature points. Owing to the explicit occurrence of $w(x) = e^{-x^2} x^2$ in Eqs. (1) and (2), a quadrature based on this weight function would appear to be a good choice and also in view of the rapid convergence of the integral in Eq. (1) noted in the preceeding section. Moreover, the quadrature points and weights $\{x_i\}$ and $\{w_i\}$ for this weight function can be scaled, that is, $W_i = s w_i e^{x_i^2} / x_i^2$ and $z_i = s x_i$ so that we have the approximation $\int_0^\infty g(x) dx \approx \sum_i W_i g(z_i)$ as used in Eq. (5). A possible concern with the solution of Eq. (2) is that the kernel $K_2(x, y)$ exhibits a cusp [2] at $x = y$; the derivative of the kernel is not continuous at this point. It is useful to notice that the linear operator defined by the left-hand-side of Eq. (2) does not have any zero eigenvalues [9] contrary to the properties of the corresponding kernels for $\ell = 0$ and 1, which have two zero eigenvalues and one zero eigenvalue, respectively.

With this quadrature procedure, a solution of the integral equation, Eq. (2), is obtained by the inversion of the set of linear algebraic equations

$$\sum_{i=1}^N W_i e^{-z_i^2} z_i^2 K_2(z_i, z_j) B(z_i) - Z(z_j) B(z_j) = -z_j^2. \tag{6}$$

The reduced viscosity is then given by

$$\varepsilon_p = \frac{16\sqrt{2}}{15} \sum_{i=1}^N W_i e^{-z_i^2} z_i^4 B(z_i). \tag{7}$$

The convergence of the solution of the Boltzmann equation obtained in this way with the scaled speed quadrature points is shown in Table 1 in comparison with the solution reported by Siewert [2]. The integrand of Eq. (1) for the viscosity is shown in the table so that we can see that the major contribution to the integral is approximately in the interval $x \in [0.4, 4.0]$. The scaling of the speed points with the parameter s is thus important so as to compute the solution in the range of x that contributes to the viscosity. With $s = 5.0/x_N$, I get the convergence of the viscosity versus the number of speed quadrature points, N, shown in Table 2. The converged results in Tables 1 and 2 are

TABLE 1. Solution of the Boltzmann equation for viscosity with speed quadrature points; $x^4 e^{-x^2} B(x)$; $(-n) \equiv \times 10^{-n}$. The last two entries in the second column for $x = 5.5$ and 6.0 are taken from Loyalka et al (2007)

x	Siewert 2002	N=20	N=30	N=40	N = 60	N=80
0.1	0.613418(-6)	0.515564(-6)	0.621236(-6)	0.612545(-6)	0.613398(-6)	0.613414(-6)
0.2	0.379213(-4)	0.385653(-4)	0.379120(-4)	0.379161(-4)	0.379207(-4)	0.379211(-4)
0.3	0.407752(-3)	0.406290(-3)	0.407632(-3)	0.407717(-3)	0.407745(-3)	0.407750(-3)
0.4	0.211391(-2)	0.211006(-2)	0.211338(-2)	0.211374(-2)	0.211387(-2)	0.211390(-2)
0.5	0.727435(-2)	0.726860(-2)	0.727258(-2)	0.727378(-2)	0.727424(-2)	0.727432(-2)
1.0	0.200043	0.199830	0.200000	0.200029	0.200040	0.200042
1.5	0.578299	0.577804	0.578200	0.578268	0.578293	0.578297
2.0	0.497222	0.496907	0.497159	0.497202	0.497219	0.497221
2.5	0.176668	0.176588	0.176651	0.176662	0.176666	0.176667
3.0	0.300107(-1)	0.300023(-1)	0.300086(-1)	0.300100(-1)	0.300105(-1)	0.300106(-1)
3.5	0.263181(-2)	0.263147(-2)	0.263168(-2)	0.263176(-2)	0.263180(-2)	0.263180(-2)
4.0	0.124651(-3)	0.124661(-3)	0.124647(-3)	0.124649(-3)	0.124650(-3)	0.124651(-3)
4.5	0.328137(-5)	0.328480(-5)	0.328135(-5)	0.328132(-5)	0.328135(-5)	0.328137(-5)
5.0	0.489457(-7)	0.488628(-7)	0.489893(-7)	0.489420(-7)	0.489467(-7)	0.489453(-7)
5.5	0.419346(-9)	0.423847(-9)	0.418882(-9)	0.418244(-9)	0.419188(-9)	0.419500(-9)
6.0	0.208417(-11)	0.209376(-11)	0.208552(-11)	0.208405(-11)	0.208450(-11)	0.208559(-11)

TABLE 2. Convergence of ε_p versus the number of speed quadrature points $s = 5.0/x_N$

N	20	30	40	60	80
ε_p	0.448816	0.448985	0.449014	0.449025	0.449027

in complete agreement with the previous results [2, 3] to the significant figures shown. Siewert [2] employed 301 "*knots*" with the Hermite cubic spline functions and a 4th order Gauss-Legendre quadrature to perform integrals over subintervals. The final integral for the viscosity, Eq. (1), was computed with 100 Gauss-Legendre quadrature points and Siewert [2] reports the value $\varepsilon_p = 0.449027806$. Sharipov and Bertoldo [4] solved the Boltzmann equation as a two dimensional problem in two velocity coordinates and used 40 grid points in each velocity direction and 200 points with a Simpson's rule to evaluate ε_p to the same precision as in Table 2. In both papers [2, 4], the size of the matrices involved is much greater than the N^2 values in Table 2 and the convergence rates were not reported. The application of the speed quadrature points and weights to this problem is very straightforward and the convergence is rapid as seen from Tables 1 and 2. The eigenvalues and eigenfunctions of the operator defined by the left-hand-side of Eq. (2) which are important for the relaxation of anistropic distributions [5]) were reported in a previous publication [9].

RELAXATION TO EQUILIBRIUM

The approach to equilibrium of a minor constituent in a background gas at equilibrium or of a single component gas are fundamental problems in kinetic theory [10, 12, 13, 14] with important current applications to trapped cold gases [15, 16]. I compare the relaxation behavior of the isotropic portion of the distribution function as determined with the Wigner-Wilkins kernel $k_0(x,y)$ [17, 18] for the linear collision operator (for unit mass ratio) and the kernel $K_0(x,y)$ for the one component gas. For the test-particle problem, there is only one zero eigenvalue corresponding to particle conservation whereas for the one component gas there are two zero eigenvalues, one for particle conservation and the other for energy conservation. For the test-particle case, detailed balance can be used to impose particle conservation so that $\lambda_0 = 0$ to machine accuracy. This can also be done for the one component gas, but then λ_1 is not zero to machine accuracy. If this eigenvalue is made zero to machine accuracy with the appropriate definition of $Z(x)$ then λ_0 is no longer exactly zero. The linear Boltzmann equation with unit mass ratio is considered in the next section. In the last section, I consider the relaxation of a small perturbation from Maxwellian for a one component gas.

TABLE 3. $T(t)/T_b$ for the Linear Boltzmann Equation with Unit Mass Ratio; $T(0)/T_b = 10$

t/N	20	40	60	80	100
0.05	8.2695	8.2573	8.2559	8.2556	8.2555
0.10	6.9389	6.9203	6.9183	6.9179	6.9178
0.15	5.9017	5.8801	5.8779	5.8774	5.8773
0.20	5.0828	5.0603	5.0581	5.0577	5.0575
0.40	3.1169	3.0985	3.0969	3.0966	3.0965
0.60	2.1982	2.1854	2.1844	2.1842	2.1842
0.80	1.7194	1.7108	1.7102	1.7101	1.7101
1.00	1.4500	1.4443	1.4439	1.4438	1.4438
1.50	1.1559	1.1536	1.1535	1.1535	1.1535

Linear Boltzmann Equation; Unit Mass Ratio

The time dependent distribution, $f(x,t)$, of a minor constituent dilutely dispersed in a second component at equilibrium is given by the Boltzmann equation

$$\frac{df(y,t)}{dt} = 2\int_0^\infty xk_0(x,y)f(x,t)dx - Z(y)f(y,t),$$ (8)

where the kernel for unit mass ratio [18] is given by

$$k_0(x,y) = \begin{cases} \sqrt{\pi}\text{erf(y)}/x & y < x \\ \sqrt{\pi}e^{x^2-y^2}\text{erf(x)}/x & y > x, \end{cases}$$ (9)

and the time scale t is in units of $[N_b\pi d^2\sqrt{kT_b/2m}]^{-1}$ where N_b and T_b are the density and temperature, respectively, of the background gas, d is the hard sphere diameter and m is the mass of the minor constituent. The kernel in Eq. (9) is usually written in reduced energy whereas in this paper reduced speed is used. This is the reason for the factor $2x$ in Eq. (8) and $2y$ in Eq. (10) below. Since particle number is conserved, there is a single eigenvalue, $\lambda_0 = 0$, of the collision operator consistent with the definition of the collision frequency as

$$Z(x) = 2\int_0^\infty yk_0(x,y)dy.$$ (10)

With the appropriate quadrature, the BE is reduced to the set of ordinary differential equations, that is,

$$\frac{df_i(t)}{dt} = 2\sum_{j=1}^N W_j z_j k_0(z_j,z_i)f_j(t) - Z_i f_i(t),$$ (11)

where $f_i(t) \equiv f(z_i,t)$ and $Z_i = 2\sum_{k=1}^N W_k z_k k_0(z_i,z_k)$. The numerical evaluation of the collision frequency rather than the use of Eq. (4) is very important so as to conserve particle number, that is $\lambda_0 = 0$ to machine accuracy. Equation (11) is integrated with a simple Euler scheme, that is,

$$f_i(t+\Delta t) = f_i(t) + \Delta t\left[2\sum_{j=1}^N W_j z_j k_0(z_j,z_i)f_j(t) - Z_i f_i(t)\right].$$ (12)

An initial Maxwellian at $T(0) > T_b$ is chosen. I show the rapid convergence of the time dependent solution of this BE with the speed quadrature method in Table 3 in terms of the temperature ratio $T(t)/T_b$ where T_b is the temperature of the background gas. The convergence is slower at the shortest times as the initial decay is controlled by the highest (eigenvalue) modes. With increasing time, the better converged lower order modes dominate the solution and the convergence improves. Although solutions of the Boltzmann equation for the hard sphere cross section have been reported previously [17], the convergence properties have not been studied. Instead of the time dependent solution obtained by a direct Euler integration of the discretized equations, the solution can be expresssed in terms of the eigenvalues and eigenfunctions. It was demonstrated in a previous paper [9], that the calculation of the eigenfunctions

TABLE 4. Approach to the Eigenvalue Continuum Boundary at $Z(0)$; WKB limit [$\exp(4\pi/\sqrt{23}) = 13.74$]; the λ_n are scaled by $Z(0)$.

n	Speed Quadrature (N = 80)	Multi-Domain (N = 96)	$\left|\frac{1-\lambda_n}{1-\lambda_{n+1}}\right|$
1	0.81902	0.8190221	
2	0.97973	0.9797339	5.526
3	0.99839	0.99838853	8.930
4	0.99988	0.99988132	12.58
5	0.99999	0.9999913460	13.58
6	1.0001	0.99999936318	13.71
7		0.999999958353	13.59
8		0.9999999926736	15.29

requires a very nonuniform grid owing to the rapid variations of the eigenfunctions near the origin in speed space, especially to resolve the discrete eigenvalues near the continuum boundary. The grid employed for this calculation is defined by the division of the semi-infinite interval into 12 sub-intervals with 8 Fejer quadrature points in each interval except the last where a shifted Laguerre quadrature is used. The interval boundaries are chosen to approximately coincide with the roots of the highest bound eigenfunction desired. The lower order eigenvalues calculated in this way are shown in comparison with the eigenvalues obtained with speed quadrature points in Table 4. The accuracy of the eigenvalues near to the continuum boundary is provided by the comparison with the asymptotic WKB result [9] as shown in the 4th column of Table 4.

Linearized Boltzmann Equation

For a one component system, I choose an initial departure from Maxwellian, that is, $f(x,0) = f_{max}(x)[1 + \phi(x,0)]$. The time dependent relaxation of $\phi(x,t)$ is given by the linearized Boltzmann equation defined by

$$\frac{\partial \phi(y,t)}{\partial t} = \int_0^\infty e^{-x^2} x^2 K_0(x,y)\phi(x,t)dx - Z(y)\phi(y,t). \tag{13}$$

The symmetric kernel in this case is the $\ell = 0$ component of the anisotropic kernel [1, 12, 13, 18] and is given by

$$K_0(x,y) = 2\sqrt{pi}[\Psi(x) - (x^3/3 + xy^2)]/(xy) \quad x < y. \tag{14}$$

with t dimensionless as defined previously. The discretized form of Eq. (13) is

$$\frac{d\phi_i(t)}{dt} = \sum_{j=1}^{N} W_j e^{-z_j^2 + z_i^2} \left(\frac{z_j}{z_i}\right)^2 K_0(z_j,z_i)\phi_j(t) - Z_i\phi_i(t), \tag{15}$$

where $\phi_i(t) \equiv \phi(z_i,t)$ and Z_i is computed analogous to that shown after Eq. (11) or alternatively with $Z_i = (2/z_i^2)\sum_{k=1}^{N} W_k z_k^4 e^{-z_k^2} K_0(z_i,z_k)$ to ensure that energy conservation is obtained to machine accuracy. In this way, one of the two zero eigenvalues is of the order of 10^{-15} but not both. The other eigenvalue is much larger of the order of 10^{-5}. The time dependence of $\phi_i(t)$ is calculated with an Euler integration of Eq. (15) analogous to Eq. (11). Energy conservation is imposed with the previously defined collision frequency and the distribution function can be renormalized at each time step. The evolution of the distribution function is shown in Fig. 1 on the left hand side and of the perturbation on the right hand side. The initial distribution, $f(x,0)$, exhibits a second peak at $x = 4$ arising from the choice of $\phi(x,0) = 4000e^{-5(x-4)^2}$. The long time form of the perturbation is a linear combination of the two eigenfunctions with zero eigenvalue, thus it is verified that $\lim_{t\to\infty} \phi(x,t) \to A + Bx^2$ which goes slightly negative for $x \approx 0$ and not visible with the scale chosen. The main peak of the distribution function moves to higher values of x with increasing time so as to maintain a constant temperature. This behaviour is in sharp contrast to the relaxation results in Table 3. A relaxation time for the approach to equilibrium can be defined with the relaxation data in Table 3. For the one component system the temperature is constant and higher order moments of the distribution could be used to define a relaxation time.

This paper has demonstrated the utility of the speed quadratures for a pseudospectral solution of three different

Boltzmann equations. Further work is in progress to study the way the cusps in the kernels affect the convergence of different numerical methods. A comparison will be made of the solution of the linearized Boltzmann equation with corresponding nonlinear Boltzmann equation [10]. A comparison with a moment method based on the matrix representation of the collision operator in the Sonine polynomial basis will also be carried out. Realistic quantum differential cross sections will also be used. Further details will appear in forthcoming publications.
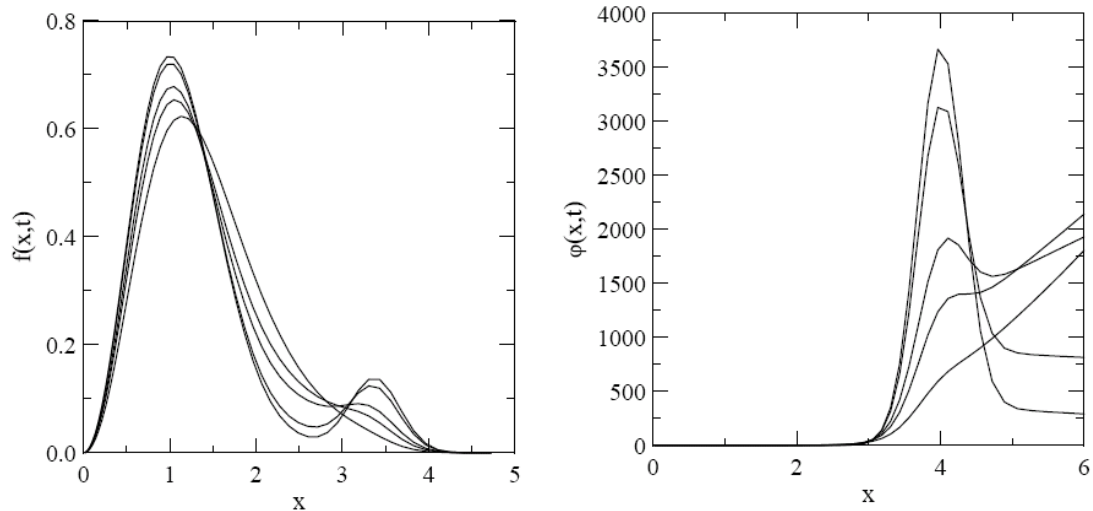

FIGURE 1. Distribution function $f(x,t) = f_{max}(x)[1 + \phi(x,t)]$; successive reduced times are $t = 0.02, 0.06, 0.2, 0.3$ and 0.5; $\phi(x,0) = 4000e^{-5(x-4)^2}$.

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