Calculation of the transport coefficients for a dilute simple gas using an iterative solution of the Boltzmann equation

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Abstract. The Chapman–Enskog second approximation to Boltzmann's equation for a dilute simple gas is obtained for several different potential models using an iterative procedure. The perturbation function to the local Maxwellian distribution, and various transport coefficients, are found as approximate sums of infinite series. Transport coefficients are calculated for Maxwellian, pseudo-Maxwellian, and rigid-sphere potential models and are compared with those obtained by the standard Chapman–Cowling method.

1. Introduction

We consider in this paper an iterative method of obtaining the distribution function and transport coefficients for a pure gas with no internal degrees of freedom, within the context of the first-order Chapman–Enskog solution to the Boltzmann equation (Chapman and Cowling 1970, chap. 7). This method has already been used with some success in analogous problems in the field of transport phenomena of electrons in metals (Jones 1969, 1971), and it is therefore of interest to see whether such an approach may also be usefully applied to transport phenomena in gases.

The iterative method is an alternative to the standard procedure introduced by Chapman and Cowling (1970, chaps 7, 9, 10), in which the first-order perturbation Φ to the distribution function is expressed as an infinite series of Sonine polynomials and the orthogonal properties of these polynomials are exploited to obtain the transport coefficients, to a good approximation, at least, by using only the first few terms in the infinite series of these polynomials.

With the iterative method, the perturbation function Φ is obtained as an infinite sum, successive terms of which are generated by successive iterations. From each term in the series we then obtain a corresponding term in the sum making up each transport coefficient. The series thus obtained are assumed to follow approximate geometrical progressions, as discussed in § 2, and the final approximations are then calculated on the basis of this assumption.

The iterative method itself is presented in § 2. In subsequent sections the method is applied to the calculation of the transport coefficients for three different potential models, the Maxwellian, pseudo-Maxwellian (soft-sphere), and rigid-sphere models.

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These particular models are chosen because they are well documented and they provide the most direct way of assessing the feasability and accuracy of the method presented in this paper. Finally, in § 5 we will discuss the results obtained.

2. Outline of iterative procedure

The Boltzmann equation for the velocity distribution function f for a single-component gas subject to no external forces has the form

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial r} = Lf \tag{1}$$

where the collision integral Lf is a functional of f, and involves the dynamics of a binary collision between molecules of the gas. The standard Chapman-Enskog solution of this equation is obtained in well known fashion (Chapman and Cowling 1970, chap. 7) as a set of successive approximations

$$f = f^{(0)} + f^{(0)}\Phi^{(1)} + f^{(0)}\Phi^{(2)} + \dots. \tag{2}$$

The first approximation $f^{(0)}$ is of Maxwellian form

$$f^{(0)} = n(m/2\pi kT)^{3/2} \exp[-m(v - u_0)^2/2kT] \tag{3}$$

with $n = n(r, t)$ the molecular number density at (r, t), $u_0 = u_0(r, t)$ the stream velocity, $T = T(r, t)$ the temperature, k the Boltzmann constant, and m the mass of a molecule. The functions $\Phi^{(N)}$ are of order N in the spatial gradients of n, u_0, and T. We wish to consider the calculation of transport coefficients for the gas, in the second approximation of Chapman and Enskog. We therefore consider the solution $\Phi^{(1)}$. This can be written (Chapman and Cowling 1970, chap. 7) as

$$f^{(0)}(V)[(\alpha V^2 - \tfrac{5}{2})V \cdot \nabla T + 2\alpha V^0 V : \nabla u_0]$$

$$= \int f^{(0)}(V)f^{(0)}(U)(\Phi^{(1)}(U') + \Phi^{(1)}(V') - \Phi^{(1)}(U) - \Phi^{(1)}(V))gb\, db\, d\epsilon\, du. \tag{4}$$

Here $U = u - u_0$, $V = v - u_0$, $\alpha = m/2kT$, $V^0 V = VV - \tfrac{1}{3}V^2\delta$ is a symmetric non-divergent tensor; u and v are the velocities of two molecules prior to collision, their velocities after collision being u' and v' respectively.

Since the left-hand side of equation (4) contains linear gradient terms in T and u_0, $\Phi^{(1)}$ may be written

$$\Phi^{(1)} = \phi_\lambda \cdot \nabla \ln T + \phi_\eta : \nabla u_0 = \phi_\lambda V \cdot \nabla \ln T + \phi_\eta V^0 V : \nabla u_0. \tag{5}$$

Substituting (5) into (4) and equating like gradients we then have

$$(\alpha V^2 - \tfrac{5}{2})V = -\phi_\lambda(V)V \int f^{(0)}(U)gb\, db\, d\epsilon\, du$$

$$+ \int f^{(0)}(U)(\phi_\lambda(V')V' + \phi_\lambda(U')U' - \phi_\lambda(U)U)gb\, db\, d\epsilon\, du \tag{6}$$

and

$$2\alpha V^0 V = -\phi_\eta(V)V^0 V \int f^{(0)}(U)gb\, db\, d\epsilon\, du$$

$$+ \int f^{(0)}(U)(\phi_\eta(V')V'^0 V' + \phi_\eta(U')U'^0 U' - \phi_\eta(U)U^0 U)gb\, db\, d\epsilon\, du \tag{7}$$

where we have used the fact that $\phi_\lambda(V)$ and $\phi_\eta(V)$ are independent of the collision operator L. For convenience we can write both (6) and (7) in the following more compact form:

$$\mathbf{X} = -\phi L_0 + L_1 \phi \tag{8}$$

where ϕ is either ϕ_λ or ϕ_η, $\mathbf{X}$ is either $(\alpha V^2 - \tfrac{5}{2})V$ or $2\alpha V^0 V$, and L_0, L_1 are the appropriate operators defined for ϕ_λ by equation (6) and for ϕ_η by equation (7).

One may solve equation (8) by iteration. The procedure may be formalised by writing

$$\phi(V) = \sum_{i=0}^{\infty} \xi^i \phi^{(i)}(V) \tag{9}$$

where ξ is a parameter eventually to be set equal to unity. Setting

$$\mathbf{X} = -\phi L_0 + \xi L_1 \phi \tag{10}$$

and equating like powers of ξ, we obtain

$$\mathbf{X}(V) = -\phi^{(0)}(V)L_0, \tag{11}$$

$$\phi^{(i)} L_0 = L_1 \phi^{(i-1)} \qquad \text{for } i \geq 1. \tag{12}$$

In these equations, ξ functions as an ordering parameter. The auxiliary conditions (Chapman and Cowling 1970, p 113) may be satisfied by demanding that they be satisfied separately for each $\phi^{(i)}$. This condition is met by using $\bar{\phi}_\lambda^{(i)}$ in place of $\phi_\lambda^{(i)}$, where

$$\bar{\phi}_\lambda^{(i)}(V)V \cdot \nabla \ln T = \phi_\lambda^{(i)}(V)V \cdot \nabla \ln T + \boldsymbol{\alpha}^{(i)} \cdot V \qquad \text{for } i \geq 0 \tag{13}$$

with $\boldsymbol{\alpha}^{(i)}$ determined by the condition

$$m \int f^{(0)}(V)\Phi^{(i)}(V)V \, dV = 0. \tag{14}$$

The heat flux q is given by

$$q = -\lambda \nabla T = \int \tfrac{1}{2}mV^2 V f^{(0)}(V)\Phi^{(1)} \, dv. \tag{15}$$

One may then obtain an iterative solution for the thermal conductivity λ by using the iterative solution for ϕ (equations (11)–(12)). One thereby obtains

$$q = -\lambda \nabla T = \tfrac{1}{2}m \int V^2 V f^{(0)}(V) \sum_{i=0}^{\infty} (\phi_\lambda^{(i)}(V)V \cdot \nabla T + \text{\textit{ffl}}\boldsymbol{\alpha}^{(i)} \cdot V) \, dV. \tag{16}$$

On writing

$$\lambda = \sum_{i=0}^{\infty} \xi^i \lambda^{(i)} \tag{17}$$

expressions for $\lambda^{(i)}$ in terms of the respective $\phi_\lambda^{(i)}$ can then be obtained.

The coefficient of shear viscosity η_s can be obtained similarly: by using the second-order correction to the pressure tensor and equations (11)–(12), one obtains

$$\mathbf{P} = -2\eta_s \nabla^s \boldsymbol{u}_0 = \tfrac{2}{15}m \int f^{(0)}(V) \sum_{i=0}^{\infty} \phi_\eta^{(i)}(V)V^4 \nabla^s \boldsymbol{u}_0 \, dv \tag{18}$$

where $\nabla^s u_0$, the shear viscosity tensor, is the symmetric non-divergent part of the tensor ∇u_0. On writing

$$\eta_s = \sum_{i=0}^{\infty} \xi^i \eta_s^{(i)}, \tag{19}$$

we can obtain expressions for $\eta_s^{(i)}$ in terms of the respective $\phi_\eta^{(i)}$'s.

In practice, the iterative procedure is used to calculate only the first few terms in (17) and (19). These terms are then assumed to form an approximate geometric progression, and approximations to the transport coefficients are determined accordingly. Thus, for instance, the first approximation to λ is taken to be

$$\lambda = \frac{\lambda^{(0)}}{1 - (\lambda^{(1)}/\lambda^{(0)})}; \tag{20}$$

it is this approximation which must be compared with the first approximation of Chapman and Cowling when comparing the two methods.

That one may expect $\lambda^{(i)}$ and $\eta^{(i)}$ to form approximate geometric progressions may be seen by writing the iterative relations (11), (12) in the form

$$\phi^{(n)} = -L_0^{-1}(L_1 L_0^{-1})^n X \qquad \text{(all } n > 0\text{).} \tag{21}$$

If X is an eigenfunction of $(L_1 L_0^{-1})$, with eigenvalue α, then

$$\phi^{(n)} = -\alpha^n L_0^{-1} X,$$

and the $\phi^{(n)}$ (and thus $\lambda^{(n)}$ and $\eta^{(n)}$) form a geometric progression. More generally, one may suppose X expanded in eigenfunctions ψ_i (supposed a complete set) of $(L_1 L_0^{-1})$ with eigenvalues α_i:

$$X = \sum_i a_i \psi_i.$$

For large n, the eigenvalue α_r of maximum modulus will dominate the sum over i, and the nth term in equation (21) will approach the value $(\alpha_r^n a_r \psi_r)$, as in a geometric progression. The corresponding term for a transport coefficient will involve integrals of ϕ in velocity space which one may expect to include a certain amount of averaging, thus enhancing the contribution of the dominant eigenfunction and making the $\lambda^{(n)}$ and $\eta^{(n)}$ even better approximations to geometric progressions than the $\phi^{(n)}$. Successive approximations are determined by the consideration that the $\lambda^{(n)}$ and $\eta^{(n)}$ are expected to approach a geometric progression more closely with increasing n. Thus, we take

$$\lambda = \lambda^{(0)} + \frac{\lambda^{(1)}}{|1 - (\lambda^{(2)}/\lambda^{(1)})|} \tag{22}$$

as the second approximation to λ.

3. Calculation of the transport coefficients for Maxwellian and pseudo-Maxwellian molecules

In this section we consider the iterative calculation of transport coefficients for intermolecular forces such that the result can be obtained analytically. We shall consider both Maxwellian and pseudo-Maxwellian molecules.

For Maxwellian molecules, the potential can be written

$$V(r) = \frac{K}{4r^4}$$

and it can easily be shown that for this potential (Chapman and Cowling 1970, p 173)

$$gb \, db = \left(\frac{K}{\mu}\right)^{1/2} \nu_0 \, d\nu_0 \qquad (23)$$

where μ is the reduced mass, and $\nu_0 = b(\mu g^2/K)^{1/4}$. Hence $gb \, db$ does not depend on g, but only on ν_0.

For pseudo-Maxwellian ('soft-sphere') molecules, the potential is given by (Koga 1970, p 229)

$$V(r) = \frac{K'}{r^{s-1}}, \qquad s \to \infty$$

with

$$K' = K'' \sigma^{s-1} (g^*/g)^{(s-1)/2}$$

where K'' and g^* are constants; then one can show that

$$gb \, db = \tfrac{1}{4}\sigma^2 g^* \sin \chi \, d\chi \qquad (24)$$

where σ is the diameter of a molecule, and χ the deflection angle. As is the case for the Maxwellian model, g disappears from the collision integrals. For this model each collision at fixed g appears like a collision between two solid spherical bodies, while if g increases, the effective molecular cross section decreases. The pseudo-Maxwellian molecules have a finite cross section while retaining all the conveniences of Maxwellian molecules; as a result, many calculations are appreciably simplified for them.

3.1. Thermal conductivity

From the zeroth iteration, equation (11), we obtain an expression for $\phi_\lambda^{(0)}$ given by

$$\phi_\lambda^{(0)}(V) V . \nabla T = \frac{(\tfrac{5}{2} - \alpha V^2) V . \nabla T}{L_0}. \qquad (25)$$

For Maxwellian and pseudo-Maxwellian molecules, the integral L_0 defined by equation (8) is velocity independent. Hence one may write

$$\phi_\lambda^{(0)}(V) = A^{(0)} + B^{(0)} \alpha V^2 \qquad (26)$$

where $A^{(0)}$ and $B^{(0)}$ do not depend on v. Performing the first iteration, equation (12), we get for $\phi_\lambda^{(1)}$

$$\phi_\lambda^{(1)} V^2 L_0 = V . L_1[(A^{(0)} + B^{(0)} V^2) V]. \qquad (27)$$

By using conservation of momentum, and standard properties of the dynamics of a collision, equation (27) can be shown to reduce to

$$\phi_\lambda^{(1)} \int gb \, db = \tfrac{5}{4} B^{(0)} \int (1 - \cos^2 \chi) gb \, db + A^{(0)} \int gb \, db + \tfrac{1}{2} B^{(0)} \alpha V^2 \int (1 + \cos^2 \chi) gb \, db$$

$$(28)$$

or

$$\phi_\lambda^{(1)} = A^{(1)} + B^{(1)}\alpha V^2 \tag{29}$$

where the angle χ is defined by figure 1. It thus follows, in general, that

$$\phi_\lambda^{(i)} = A^{(i)} + B^{(i)}\alpha V^2 \tag{30}$$

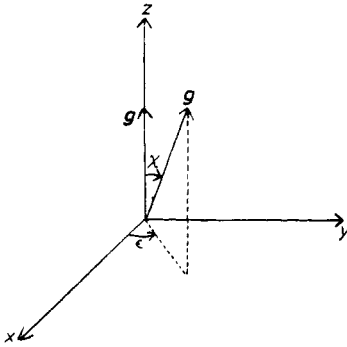where $A^{(i)}$ and $B^{(i)}$ are independent of V.

Figure 1.

In order to satisfy the auxiliary conditions, one must instead of $\phi_\lambda^{(i)}$ use the re-defined perturbation function $\bar\phi_\lambda^{(i)}$ of equation (13); the factor $\alpha^{(i)}$ in this equation is determined by equation (14), and one finds that

$$\alpha^{(i)} = -(A^{(i)} + \tfrac{5}{2}B^{(i)})\frac{\nabla T}{T}.$$

Thus, we obtain from equations (13) and (30) that

$$\bar\phi_\lambda^{(i)}V \cdot \frac{\nabla T}{T} = (\alpha V^2 - \tfrac{5}{2})B^{(i)}V \cdot \frac{\nabla T}{T}. \tag{31}$$

As already stated, it is the $\bar\phi^{(i)}$ rather than the $\phi^{(i)}$ which obey all the auxiliary conditions and are consequently used in the calculation of $\lambda^{(i)}$.

From equations (28), (29), and (30) we can write

$$B^{(i+1)} = \tfrac{1}{2}B^{(i)}\frac{\int (1+\cos^2\chi)gb\,db}{\int gb\,db}. \tag{32}$$

Equation (32) shows that the $B^{(i)}$ are described by a geometrical progression whose sum is given by

$$B = \sum_{i=0}^{\infty} B^{(i)} = \frac{B^{(0)}}{1-(B^{(1)}/B^{(0)})}$$

with

$$B^{(0)} = -\frac{1}{\int f^{(0)}(U)gb\,db\,d\epsilon\,d\boldsymbol{u}} = -\frac{1}{2\pi n\int gb\,db};$$

therefore

$$B = -\frac{1}{n\pi \int (1 - \cos^2 \chi) gb \, db}.$$ (33)

The coefficient of thermal conductivity λ can then be obtained from the heat flux, equation (16), and one has

$$\lambda = -\frac{5Bnk^2T}{2m}.$$ (34)

Finally we have to consider the form of B for the respective models.

In calculating B from equation (33), for Maxwellian molecules, one uses equation (22) and the definition

$$A_l(5) = \int_0^\infty (1 - \cos^l \chi) \nu \, d\nu_0.$$

Values for $A_2(5)$ needed here are given in the literature (Chapman and Cowling 1970, p 172). One thus obtains

$$B = -\frac{1}{n\pi A_2(5)} \left(\frac{m}{2K}\right)^{1/2}$$

and (35)

$$\lambda = \frac{5}{2\pi} \frac{k^2T}{(2mK)^{1/2}A_2(5)}.$$

This result agrees with the value of λ obtained in the usual way (Chapman and Cowling 1970, p 174).

For the pseudo-Maxwellian or soft-sphere model, from equation (24), equation (33) for B becomes

$$B = -\frac{3}{n\pi\sigma^2 g^*}$$

while λ is given by (36)

$$\lambda = \frac{15}{2\pi} \frac{k^2T}{m\sigma^2 g^*}.$$

This result agrees with the value of λ obtained by the standard calculation (Koga 1970, p 230).

3.2. Viscosity

From the zeroth iteration, equation (11), we have

$$\phi_\eta^{(0)}(V) V^0 V : \nabla u_o = -\frac{2\alpha V^0 V : \nabla u_0}{L_0}.$$ (37)

This is of the form

$$\phi_\eta^{(0)}(V) V^0 V : \nabla u_0 = D^{(0)} V^0 V : \nabla u_0$$ (38)

where $D^{(0)}$ does not depend on V. As for the thermal conductivity case, we expect a generalisation of the form

$$\phi_\eta^{(i)}(V)V^0V:\nabla u_0 = D^{(i)}V^0V:\nabla u_0. \tag{39}$$

This is indeed the case. Following the method used for $B^{(i)}$'s we obtain the relationship

$$D^{(i+1)} = \tfrac{1}{4}D^{(i)}\frac{\int(1+3\cos^2\chi)gb\,\mathrm{d}b}{\int gb\,\mathrm{d}b}. \tag{40}$$

Equation (40) shows that the $D^{(i)}$ are described by a geometrical progression whose sum is given by

$$D = \sum_{i=0}^{\infty}D^{(i)} = \frac{D^{(0)}}{1-(D^{(1)}/D^{(0)})}$$

or $\tag{41}$

$$D = -\frac{4\alpha}{3\pi n\int(1-\cos^2\chi)gb\,\mathrm{d}b}.$$

The coefficient of viscosity η can then be obtained from equation (18) for the pressure tensor. One obtains

$$\eta_s = -D\frac{nk^2T}{m}. \tag{42}$$

Finally, we have to evaluate D for the models under consideration.

For Maxwellian molecules we have from equation (23) that

$$D = -\frac{4\alpha}{3\pi nA_2(5)}\left(\frac{m}{2K}\right)^{1/2}.$$

Hence η_s is given by

$$\eta_s = \frac{1}{3}\left(\frac{2m}{K}\right)^{1/2}\frac{kT}{\pi A_2(5)}. \tag{43}$$

This result agrees with the value of η_s obtained by the standard calculation (Chapman and Cowling 1970, p 174).

For the soft-sphere model, we obtain from equation (24) the expression for D:

$$D = -\frac{4\alpha}{\pi n\sigma^2 g^*}.$$

Hence the coefficient of viscosity is given by

$$\eta_s = \frac{2kT}{\pi\sigma^2 g^*}. \tag{44}$$

This is the same as the value of η_s obtained by the standard Chapman–Enskog method (Koga 1970, p 230).

4. Rigid-sphere potential model

The potential for rigid-sphere molecules may be written (Kogo 1970, p 228)

$$V(r) = \frac{\bar{K}}{r^{s-1}}, \qquad s \to \infty$$

with $\bar{K} = \bar{K}'\sigma^{s-1}$; then one can show that for this model

$$b \, db = \tfrac{1}{4}\sigma^2 \sin \chi \, d\chi. \tag{45}$$

Hence the collision integral is g-dependent; in consequence, the analysis to be performed is more complex than for the Maxwellian case, and the final integrals will be evaluated numerically.

4.1. Thermal conductivity

We use the iterative procedure of equations (11) and (12), together with equation (6), to obtain the relations

$$(\tfrac{5}{2} - \alpha V^2)V = \phi_\lambda^{(0)}(V)V \int f^{(0)}(U)gb \, db \, d\epsilon \, d\boldsymbol{u}$$

and

$$\phi_\lambda^{(i)}(V)V \int f^{(0)}(U)gb \, db \, d\epsilon \, d\boldsymbol{u}$$

$$= \int f^{(0)}(U)(\phi_\lambda^{(i-1)}(V')V'\hat{\boldsymbol{V}}' \cdot \hat{\boldsymbol{V}} + \phi_\lambda^{(i-1)}(U')U'\hat{\boldsymbol{U}}' \cdot \hat{\boldsymbol{V}}$$

$$- \phi_\lambda^{(i-1)}(U)U\hat{\boldsymbol{U}} \cdot \hat{\boldsymbol{V}})gb \, db \, d\epsilon \, d\boldsymbol{u}. \tag{46}$$

The integrals are then manipulated using methods similar to those of Brooker and Green (1968), and the equations (46) can be shown to reduce to

$$\phi_\lambda^{(0)}(V) = (\tfrac{5}{2} - \alpha V^2)\left\{4\pi^2\sigma^2\left(\frac{\alpha}{\pi}\right)^{3/2} n\left[\int_0^V U^2 e^{-\alpha U^2}\left(\frac{\tfrac{1}{3}U^3 + UV^2}{UV}\right) du\right.\right.$$

$$\left.\left. + \int_V^\infty U^2 e^{-\alpha U^2}\left(\frac{\tfrac{1}{3}V^3 + VU^2}{UV}\right) du\right]\right\}^{-1} \tag{47}$$

for $\phi_\lambda^{(0)}$ and

$$\phi_\lambda^{(1)}(V) = \left\{\frac{8\pi^2\sigma^2}{\alpha}\int_0^V \phi_\lambda^{(0)}(U)U^3\left[\int_0^U e^{-\alpha y^2}\left(\frac{U^2 - 2y^2}{U^2 V^2}\right) dy\right] dU\right.$$

$$+ \frac{8\pi^2\sigma^2}{\alpha}\int_V^\infty \phi_\lambda^{(0)}(U)U^3 e^{-\alpha(U^2 - V^2)}\left[\int_0^V e^{-\alpha y^2}\left(\frac{V^2 - 2y^2}{U^2 V^2}\right) dy\right] dU$$

$$- 4\pi^2\sigma^2\int_0^V U^3 e^{-\alpha U^2}\phi_\lambda^{(0)}(U)\frac{V}{3}\left[\frac{1}{5}\left(\frac{U}{V}\right)^3 - \left(\frac{U}{V}\right)\right] dU$$

$$\left. - 4\pi^2\sigma^2\int_V^\infty U^3 e^{-\alpha U^2}\phi_\lambda^{(0)}(U)\frac{U}{3}\left[\frac{1}{5}\left(\frac{V}{U}\right)^3 - \left(\frac{V}{U}\right)\right] dU\right\}$$

$$\times \left\{ 4\pi^2 \sigma^2 V \left[\int_0^V U^2 \, e^{-\alpha U^2} \left(\frac{\frac{1}{3}U^3 + UV^2}{UV} \right) dU \right. \right.$$

$$\left. \left. + \int_V^\infty U^2 \, e^{-\alpha U^2} \left(\frac{\frac{1}{3}V^3 + U^2 V}{UV} \right) dU \right] \right\}^{-1} \tag{48}$$

for $\phi^{(1)}$. Additional mathematical details may be found in Martin (1972).

Because of the difficulty associated with the computation of multiple integrals, one is in practice restricted to the calculation of the first few terms in ϕ. The present work will not be carried beyond the calculation of $\phi_\lambda^{(2)}$.

From equations (16) and (17), λ is given as the sum of an infinite set of $\lambda^{(i)}$, where each $\lambda^{(i)}$ is obtained from a corresponding $\phi_\lambda^{(i)}$. The relation reduces to

$$\lambda^{(i)} = \frac{2}{3} \frac{mn\pi}{\alpha T} \left(\frac{\alpha}{\pi} \right)^{3/2} \int_0^\infty (\tfrac{5}{2} - \alpha V^2) \phi_\lambda^{(i)}(V) V^4 \, dV \tag{49}$$

upon performing the angular integrations. Assuming that the $\lambda^{(i)}$ follow an approximate geometric progression, we then obtain successive approximations to λ following equations (20) and (22).

We use the numerical values of $\phi_\lambda^{(0)}$ obtained from equation (47) to obtain $\lambda^{(0)}$ from the numerical integration of equation (49). We obtain

$$\lambda^{(0)} = \frac{1}{\sigma^2} \left(\frac{k^3 T}{\pi m} \right)^{1/2} (0.48681 \pm 3 \times 10^{-5}), \tag{50}$$

which is about 40% of the value of the fourth approximation $[\lambda]_4$ obtained by Chapman and Cowling (1970, p 169); $[\lambda]_4$ may be considered 'exact' for present purposes. $\lambda^{(1)}$ is calculated similarly, and one obtains

$$\lambda^{(1)} = \frac{1}{\sigma^2} \left(\frac{k^3 T}{\pi m} \right)^{1/2} (0.2786 \pm 1 \times 10^{-4}). \tag{51}$$

The assumption that the $\lambda^{(i)}$ follow an approximate geometrical progression then gives us the first approximation to λ using equation (20),

$$\lambda = \frac{1}{\sigma^2} \left(\frac{k^3 T}{\pi m} \right)^{1/2} (1.1384 \pm 2 \times 10^{-4}). \tag{52}$$

The value obtained is a good approximation, about 95% of the value for $[\lambda]_4$. The $\lambda^{(2)}$ term is calculated similarly; the result is

$$\lambda^{(2)} = \frac{1}{\sigma^2} \left(\frac{k^3 T}{\pi m} \right)^{1/2} (0.169 \pm 2 \times 10^{-3}). \tag{53}$$

On comparing the ratios $\lambda^{(1)}/\lambda^{(0)} = 0.5724 \pm 2 \times 10^{-4}$ and $\lambda^{(2)}/\lambda^{(1)} = 0.605 \pm 9 \times 10^{-3}$, it can be seen that they do not differ much, about 3–7%. This is consistent with the supposition that the $\lambda^{(i)}$'s form an approximate geometrical progression.

The second approximation to λ is obtained from equation (22) (this corresponds to using the Padé approximation [1, 1]). This result is

$$\lambda = \frac{1}{\sigma^2} \left(\frac{k^3 T}{\pi m} \right)^{1/2} (1.192 \pm 0.016) \tag{54}$$

which is equivalent to $(99.2 \pm 1.3)\%$ of the value $[\lambda]_4$. (If we had used the Padé

approximation [0, 2], we would have obtained an answer which is 99% of that obtained by the standard method).

4.2. Calculation of the coefficient of viscosity

The calculation of the coefficient of viscosity by the iterative method is similar to that for thermal conductivity. We use equation (7) together with the iterative procedure of equations (11) and (12), and reduce the resulting integrals by methods similar to those of Brooker and Green (1968) to integrals suitable for numerical calculation. The relations may be shown to reduce to

$$
\phi_n^{(0)}(V) = -2\alpha \Big\{ 4\pi^2\sigma^2 n \Big(\frac{\alpha}{\pi}\Big)^{3/2} \Big[\int_0^V U^2 e^{-\alpha U2} \Big(\frac{\frac{1}{3}U^3 + UV^2}{UV}\Big) du
$$
$$
+ \int_V^\infty U^2 e^{-\alpha U2} \Big(\frac{\frac{1}{3}V^3 + VU^2}{UV}\Big) du \Big] \Big\}^{-1} \tag{55}
$$

for $\phi_n^{(0)}$ and

$$
\phi_n^{(1)}(V) = \frac{2}{\alpha V^2} \Big[\int_0^V \phi_n^{(0)}(U) U^4 \Big(\frac{3}{2}\int_0^U \frac{1}{U^3V^3}(U^4 + 4y^4 - 5U^2y^2 + V^2y^2) e^{-\alpha y2}\, dy
$$
$$
- \frac{1}{2}\int_0^U \frac{1}{UV} e^{-\alpha y2}\, dy \Big)\, du + \int_V^\infty \phi_n^{(0)}(U) U^4 e^{-\alpha(U2-V2)}
$$
$$
\times \Big(\frac{3}{2}\int_0^V \frac{1}{U^3V^3}(V^4 + 4y^4 - 5V^2y^2 + U^2y^2) e^{-\alpha y2}\, dy
$$
$$
- \frac{1}{2}\int_0^V \frac{1}{UV} e^{-\alpha y2}\, dy \Big)\, du \Big] \Big[\int_0^V U^2 e^{-\alpha U2} \Big(\frac{\frac{1}{3}U^3 + UV^2}{UV}\Big)\, du
$$
$$
+ \int_V^\infty U^2 e^{-\alpha U2} \Big(\frac{\frac{1}{3}V^3 + U^2V}{UV}\Big)\, du \Big]^{-1}
$$
$$
+ \Big[\int_0^V e^{-\alpha U2}\phi_n^{(0)}(U) U^4 \Big(\frac{U^4}{7V^3} - \frac{U^2}{3V}\Big)\, du
$$
$$
+ \int_V^\infty e^{-\alpha U2}\phi_n^{(0)}(U) U^4 \Big(\frac{V^4}{7U^3} - \frac{V^2}{3U}\Big)\, du \Big]
$$
$$
\times \Big\{ 5V^2 \Big[\int_0^V e^{-\alpha U2} U^2 \Big(\frac{\frac{1}{3}U^3 + UV^2}{UV}\Big)\, du
$$
$$
+ \int_V^\infty e^{-\alpha U2} U^2 \Big(\frac{\frac{1}{3}V^3 + U^2V}{UV}\Big)\, du \Big] \Big\}^{-1} \tag{56}
$$

for $\phi_n^{(1)}$.

The terms $\eta_s^{(i)}$ in the expression (19) for the coefficient of viscosity η_s are obtained from equation (18) for the pressure tensor,

$$
\eta_s^{(i)} = -\frac{4\pi m n}{15} \Big(\frac{\alpha}{\pi}\Big)^{3/2} \int_0^\infty \phi_n^{(i)}(V) e^{-\alpha V2} V^6\, dV \tag{57}
$$

evaluated numerically. The present work is not carried beyond calculation of $\eta_s^{(2)}$.

The final results for $\eta_s^{(0)}$, $\eta_s^{(1)}$ and $\eta_s^{(2)}$ are:

$$\eta_s^{(0)} = \frac{0 \cdot 1972}{\sigma^2}\left(\frac{kmT}{\pi}\right)^{1/2} \tag{58}$$

$$\eta_s^{(1)} = \frac{0 \cdot 0627}{\sigma^2}\left(\frac{kmT}{\pi}\right)^{1/2} \tag{59}$$

$$\eta_s^{(2)} = \frac{0 \cdot 0254}{\sigma^2}\left(\frac{kmT}{\pi}\right)^{1/2}. \tag{60}$$

The value of $\eta_s^{(0)}$ is about 62% of the value of the fourth approximation $[\eta_s]_4$ of Chapman and Cowling (1970, p 169); the latter value may be assumed 'exact' for present purposes.

The first approximation to η_s is obtained from the values (58) and (59), together with the assumption that the $\eta_s^{(i)}$ form a geometrical progression, so that

$$\eta_s = \frac{\eta_s^{(0)}}{1 - (\eta_s^{(1)}/\eta_s^{(0)})}.$$

We obtain

$$\eta_s = \frac{0 \cdot 2891}{\sigma^2}\left(\frac{kmT}{\pi}\right)^{1/2}. \tag{61}$$

The value of η_s obtained here is a good approximation, being about 91% of the value $[\eta_s]_4$. The second approximation uses equation (60) and the relation

$$\eta_s = \eta_s^{(0)} + \frac{\eta_s^{(1)}}{|1 - (\eta_s^{(2)}/\eta_s^{(1)})|}.$$

The result is

$$\eta_s = \frac{0 \cdot 3026}{\sigma^2}\left(\frac{kmT}{\pi}\right)^{1/2} \tag{62}$$

which is equivalent to 95·3% of the value $[\eta_s]_4$.

5. Conclusions

The iterative method gives solutions for the pure gas coefficients of thermal conductivity, λ, and viscosity, η_s, as well as the solution for the first-order perturbation $\Phi^{(1)}$ to the equilibrium distribution function $f^{(0)}$, equation (2), within the context of the first-order Chapman–Enskog solution to the Boltzmann equation (Chapman and Cowling 1970, chap. 7).

For the Maxwellian and pseudo-Maxwellian models the $\phi^{(i)}$ and hence $\lambda^{(i)}$'s and $\eta^{(i)}$'s form an exact geometrical progression which can be summed, and the analytic values for the transport coefficients are the same as obtained by the standard Chapman–Enskog method. One also obtains the exact solutions for the $\phi^{(i)}$.

For a pure gas of hard spheres, we have found values for the transport coefficients which are good approximations to their exact values. The first and second approximations to λ, equations (52) and (54), give values of 0·948, and 0·992, of the exact value; the corresponding approximations to η_s are 0·911 and 0·953 of the exact value.

This example is one in which the standard Chapman–Cowling method of calculation is known to converge rapidly (Chapman and Cowling 1970, chap. 10). The Chapman–Cowling first and second approximations to λ are 0·975, and 0·998, of the exact value, the corresponding approximations to η_s being 0·984, and 0·999, of the exact value. The Chapman–Cowling scheme provides a somewhat better approximation to the transport coefficients, order for order, giving a better approximation to the coefficient of viscosity than to the coefficient of thermal conductivity. The iterative procedure is also seen to give very good approximations to the transport coefficients, and appears to be particularly good in the calculation of the coefficient of thermal conductivity.

There are circumstances in which the Chapman–Cowling method is known to converge more slowly, for instance in the case of a gas mixture in which the molecular masses of the component species differ greatly from each other. For cases such as this, we suggest that the iterative method may provide a useful alternative to the usual Chapman–Cowling procedure for calculating transport coefficients.

The iterative method has been extended to deal with binary gas mixtures. This work will be presented in a subsequent paper.

Acknowledgments

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