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Model equations in the kinetic theory of gases

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Abstract. The Boltzmann transport equation cannot be solved exactly, even after it is linearized by assuming that the deviation from equilibrium is small. A number of authors have studied model equations, obtained by replacing the (linearized) collision term in the Boltzmann equation by various simpler linear operators. These 'model' operators are of finite rank and are bounded. The hope is that exact solutions of such model equations can be used to deduce qualitative features of the exact solutions of the Boltzmann equation.

We propose an alternative model, no less realistic in most respects than the usual ones, which leads to physical conclusions which are the exact opposites of the results in the literature. In particular, with our model all normal modes have normalizable eigenfunctions, and the eigenvalues are analytic functions of the wavenumber k for all k . No so called 'Knudsen modes' exist in our model.

Qualitative arguments are given to suggest that the difference results from the fact that our model operator, like the true Boltzmann collision operator, is unbounded, whereas the conventional model operators are bounded.

1. Introduction

Consider a box of volume V , containing N gas atoms, each of mass m . If the gas is in equilibrium at temperature T , then the distribution function $f(\mathbf{r}, \mathbf{c}, t)$ is independent of position \mathbf{r} and time t and has the form:

$$f_0(\mathbf{r}, \mathbf{c}, t) = (N/V)\pi^{-3/2} \exp(-c^2) \quad (1.1)$$

where \mathbf{c} is related to the velocity \mathbf{v} by (k is Boltzmann's constant)

$$\mathbf{c} = (m/2kT)^{1/2}\mathbf{v}. \quad (1.2)$$

For non-equilibrium states, $f(\mathbf{r}, \mathbf{c}, t)$ depends on \mathbf{r} and t , as well as on \mathbf{c} ; the Boltzmann equation is linearized by writing

$$f = f_0(1+h) = f_0 + f_1 \quad (1.3)$$

and assuming that f_1 , the deviation from the equilibrium distribution, is small enough so that terms quadratic in f_1 can be ignored. The resulting equation has the form:

$$\partial f_1 / \partial t + \mathbf{c} \cdot (\partial f_1 / \partial \mathbf{r}) = Lf_1 \quad (1.4)$$

where L is a linear operator which acts only on the velocity variable in f_1 . The operator L has a five-fold degenerate eigenvalue zero, and is otherwise negative definite. A full discussion of the spectrum of L is possible for so called 'Maxwell molecules', ie, molecules

repelling each other with an inverse fifth-power force law. For such molecules the eigenvalue equation

$$Lu_{\alpha}(c) = \mu_{\alpha}u_{\alpha}(c) \tag{1.5}$$

can be solved exactly. The eigenfunctions are the so called Burnett functions (known in quantum mechanics as eigenfunctions of the three-dimensional isotropic linear harmonic oscillator); the first five eigenvalues μ_{α} , $\alpha = 1, 2, 3, 4, 5$, are zero; all other eigenvalues are real and negative, and go to $-\infty$ for large values of $n + l$ in the composite index $\alpha = (n, l, m)$ of the Burnett function $u_{nlm}(c)$.

Since (1.4) is invariant under translations in r and t , it can be discussed by means of the *ansatz*:

$$f_1(r, c, t) = \exp(i\mathbf{k} \cdot \mathbf{r} + \lambda t)\phi(c) \tag{1.6}$$

which leads to the k -dependent eigenvalue problem

$$(L - i\mathbf{k} \cdot c)\phi(c) = \lambda\phi(c). \tag{1.7}$$

In the limit of small wavevectors k this reduces to (1.5). One therefore expects that the eigenvalues $\lambda_{\alpha}(k)$ have the property:

$$\lim_{k \rightarrow 0} \lambda_{\alpha}(k) = \mu_{\alpha}. \tag{1.8}$$

If this is true, exactly five eigenvalues approach zero in that limit; these are the ‘macroscopic modes’, interpreted as heat conduction (one mode), sound wave propagation (two modes), and dissipation of shear motion (two modes). For a detailed discussion, see Wang Chang and Uhlenbeck (1952) and Foch and Ford (1970). All other modes are ‘microscopic’, decaying with lifetimes comparable to $(-\mu_{\alpha})^{-1}$; these lifetimes are of the order of the mean free time of a gas atom between successive collisions with other gas atoms. A mode with real negative λ_{α} is a purely dissipative mode; oscillatory modes are associated with two eigenvalues λ_{α} which are complex conjugates of each other; the (negative) real part gives the rate of dissipation, the imaginary part gives the circular frequency $\omega_{\alpha}(k)$.

Unfortunately, an exact discussion of the eigenvalue problem (1.7) is impossible, even for Maxwell molecules; for more realistic molecular models, even (1.5) cannot be solved exactly, to say nothing of (1.7).

Wang Chang and Uhlenbeck (1952) pioneered an approximation method which goes as follows: $\phi(c)$ in (1.7) is expanded in a series of Burnett functions, and this series is truncated after a finite number K of terms. The matrix elements of L with respect to Burnett functions can be determined quite generally (Aisbett *et al* 1974), and were known in particular cases a long time ago; the matrix elements of the operator c are easy to find. The truncated problem then reduces to the algebraic problem of determining the eigenvalues and eigenvectors of a known $K \times K$ matrix. This can be done analytically for small values of k , and generally for all k by numerical methods. It is assumed that all but perhaps the final few of the K eigenvalues so found are close to the corresponding eigenvalues of the exact problem. The method works well, apparently, for small k , but runs into practical difficulties for large k (meaning $|k| \gtrsim \Lambda^{-1}$, where Λ is the mean free path of a gas atom).

However, such a truncation method is inherently incapable of finding a continuous part of the eigenvalue spectrum in (1.7), even if a continuous spectrum exists. A continuous spectrum is associated with eigenfunctions which are not properly normalizable

functions but rather are distributions, ie, they contain delta-function parts. No truncated expansion can represent such a distribution, and thus a continuous spectrum is excluded from the start by the approximation method.

It is of interest, therefore, to study exact solutions of model equations similar to (1.7), obtained from (1.7) by replacing the Boltzmann collision operator L by some simpler 'model' operator L_0 , say, chosen so that (1.7) is exactly soluble, and yet, hopefully, so that L_0 is in some qualitative sense still similar to L . The first such model was proposed by Bhatnagar *et al* (1954); for recent references, we refer to McCormack (1973).

The results from these studies are startling: according to Foch and Ford (1970), only the five 'macroscopic' modes are genuine. *All* other modes found by the truncation method are spurious! Even the five macroscopic modes exist only for sufficiently small wavenumbers k ; beyond some limiting k value, the macroscopic modes disappear altogether, and all modes are 'Knudsen modes', ie, they contain delta-function parts within $\phi(c)$. Furthermore, there is no functional relationship between λ and k for Knudsen modes: there is a continuous range of λ values for any one value of k .

In § 2 we indicate, by means of a model even simpler than that of Foch and Ford, just how these Knudsen modes arise. In § 3 we present an alternative model, no less realistic than that of § 2, which leads to exactly opposite physical conclusions. These results are discussed in § 4.

2. A simplified model with a bounded operator

For our purposes, we can restrict ourselves to one-dimensional models. The vectors r and c are replaced by scalars x and c , respectively, so that (1.4) becomes:

$$\partial f_1 / \partial t + c(\partial f_1 / \partial x) = L f_1. \quad (2.1)$$

The Burnett functions are replaced by parabolic cylinder functions (Whittaker and Watson 1950, see paragraphs 16.5 to 16.7), which are Hermite polynomials multiplied by $\exp(-c^2)$:

$$\begin{aligned} u_n(c) &= (2/\pi)^{1/4} (n!)^{-1/2} D_n(2c) \\ &= (2/\pi)^{1/4} (n!)^{-1/2} \left(-\frac{1}{2}\right)^n \exp(+c^2) \frac{d^n}{dc^n} \exp(-2c^2). \end{aligned} \quad (2.2)$$

These functions are normalized by:

$$\int_{-\infty}^{\infty} u_n(c) u_m(c) dc = \delta_{nm} \quad (2.3)$$

and the leading member of the set is

$$u_0(c) = (2/\pi)^{1/4} \exp(-c^2). \quad (2.4)$$

Our super-simplified model operator L_0 is constructed so as to be equivalent to multiplication by a negative real constant $-q$ for all functions except the function u_0 ; when L_0 operates on u_0 , it gives zero:

$$L_0 u_n(c) = \begin{cases} 0 & \text{for } n = 0 \\ -q u_n(c) & \text{for } n \geq 1. \end{cases} \quad (2.5)$$

The explicit form of the operator L_0 is

$$L_0\phi = -q\phi + qu_0(c) \int_{-\infty}^{\infty} u_0(c')\phi(c') dc' \quad (2.6)$$

The one-dimensional analogue of (1.7) is

$$(L - ikc)\phi(c) = \lambda\phi(c). \quad (2.7)$$

When L_0 , (2.6), is substituted for L in (2.7), the result can be written in the form

$$ik(c - w)\phi(c) = qu_0(c) \int_{-\infty}^{\infty} u_0(c')\phi(c') dc' \quad (2.8a)$$

$$w = i(\lambda + q)/k. \quad (2.8b)$$

We note that the right-hand side of (2.8a) is a constant multiple of the known function $u_0(c)$. We also note that w is a constant, from which the eigenvalue λ can be deduced by (2.8b).

This is enough to show just how the 'Knudsen modes' arise in such a model. The discussion of (2.8) depends completely on whether w , (2.8b), is a real number, or has a nonzero imaginary part. If the imaginary part of w is nonzero, the factor $c - w$ on the left-hand side of (2.8a) can never vanish for any real value of the variable c . We can therefore divide by $c - w$ to get the explicit form

$$\phi(c) = Au_0(c)/(c - w) \quad w \text{ complex} \quad (2.9)$$

where A is an arbitrary constant. Substitution of (2.9) into (2.8a) leads to a consistency condition, which in turn restricts w , and hence λ , to specific eigenvalues. The function (2.9) is a proper, normalizable function.

On the other hand, if w is purely real, division by $c - w$ causes trouble when $c = w$. The form of the solution is now:

$$\phi(c) = AP[u_0(c)/(c - w)] + B\delta(c - w) \quad w \text{ real} \quad (2.10)$$

where A and B are constants, $\delta(c - w)$ is the Dirac delta-function, and the symbol 'P' indicates that the principal value must be taken in any integration over c which includes the point $c = w$ within the interval of integration. Further discussion shows that the constants A and B are inter-related, so only one of them is free. However, another completely free parameter is now present, namely the (real) value of w . It turns out that (2.10) gives a solution of (2.8), in terms of distributions rather than functions but still consistent, no matter what value of w we choose.

This covers the essential points. The details are so completely similar to the ones discussed by Foch and Ford (1970) that we refer to their work, with an extremely similar model, and merely state the conclusions. These are:

(i) All but a finite number of modes are distributions rather than normalizable functions. For these so called 'Knudsen modes', there exists no functional relation between λ and k ; rather:

$$\lambda = -q - ikw \quad (2.11)$$

so that the imaginary part of λ is completely arbitrary, for all k except $k = 0$.

(ii) There is a limiting value k_{\max} , such that for $k > k_{\max}$ all modes are Knudsen modes. In our model, we find $k_{\max} = (2\pi)^{1/2}q$; Foch and Ford find $k_{\max} = 1.95q$ for their model.

(iii) For sufficiently small values of k there do exist a finite number of modes with normalizable $\phi(c)$ and such that λ is a function of k . The number of these ordinary modes equals the degeneracy of the eigenvalue $\mu = 0$ of the operator L in (2.1).

(iv) In our model, there is exactly one ordinary mode, with real negative $\lambda(k)$. It corresponds to the decay of density fluctuations by self-diffusion, rather than to sound waves. Foch and Ford get two ordinary modes with their model, corresponding physically to sound waves.

Foch and Ford (1970) suggest that conclusions (i)–(iii) also apply to the Boltzmann equation, so that all but the five macroscopic modes are of the Knudsen type, and even the five macroscopic modes disappear at sufficiently high wavenumbers.

3. A simplified model with an unbounded operator

We define an alternative model operator, L_1 , to have the same eigenfunctions $u_n(c)$ as before, but different eigenvalues:

$$L_1 u_n(c) = \mu_n u_n(c) \tag{3.1}$$

$$\mu_n = -4n \quad n = 0, 1, 2, 3, \dots \tag{3.2}$$

Just like L_0 , (2.5), the operator L_1 has exactly one zero eigenvalue, with eigenfunction $u_0(c)$, and all other eigenvalues are negative. Unlike L_0 , the operator L_1 is not bounded, ie, the eigenvalues can become infinitely large in absolute value. It is interesting to observe that the same is true of the Boltzmann collision operator for Maxwell molecules (see Wang Chang and Uhlenbeck 1952).

A linear operator is defined uniquely by its eigenfunctions and eigenvalues, so L_1 is defined by (3.1) and (3.2). Fortunately, L_1 allows an extremely simple representation as a *differential operator*, namely:

$$L_1 = \frac{d^2}{dc^2} - 4c^2 + 2. \tag{3.3}$$

The proof that (3.3) leads to (3.1) and (3.2) is simply a restatement of the standard theory of the linear harmonic oscillator in quantum mechanics. Compared to the linear harmonic oscillator Hamiltonian of quantum mechanics, L_1 differs only trivially: the sign has been changed, to make L_1 negative rather than positive, and the +2 has been added to force the leading eigenvalue to zero.

Substitution of L_1 into (2.7) leads to the differential equation:

$$\phi''(c) = (4c^2 + ikc + \lambda - 2)\phi(c). \tag{3.4}$$

This can be simplified by a shift of origin in the complex c plane. Define:

$$z = c + (ik/8) \tag{3.5}$$

to get

$$d^2\phi/dz^2 = (4z^2 + \frac{1}{16}k^2 + \lambda - 2)\phi(z). \tag{3.6}$$

This is directly related to Weber's equation (see Whittaker and Watson 1950, chap 16). If we define s by

$$s = -\frac{1}{4}(\lambda + \frac{1}{16}k^2) \tag{3.7}$$

then the solutions of (3.6) can be expressed in terms of the parabolic cylinder functions $D_s(2z)$ and $D_s(-2z)$. Returning to the original variables, we get :

$$\phi(c) = AD_s(2c + \frac{1}{4}ik) + BD_s(-2c - \frac{1}{4}ik) \tag{3.8}$$

as the general solution of (3.4), with two arbitrary constants A and B .

For arbitrary complex s , Whittaker and Watson give the detailed asymptotic behaviour of $D_s(z)$ for large $|z|$. It is trivially easy to check that the function (3.8) becomes infinite like $\exp(+c^2)$ either for large positive c , or for large negative c , or for both, for all complex values of s except the eigenvalues :

$$s = n = 0, 1, 2, 3, \dots \tag{3.9}$$

for which the eigenfunctions are (except for normalization)

$$\phi_n(c) = D_n(2c + \frac{1}{4}ik). \tag{3.10}$$

Substitution of (3.9) into (3.7) yields

$$\lambda_n(k) = -4n - (k^2/16). \tag{3.11}$$

This finishes the mathematics. The physical conclusions are :

- (i) All normal modes have ordinary, normalizable eigenfunctions. There are no Knudsen modes.
- (ii) There is no upper limit on k .
- (iii) The number of ordinary modes is infinite, and their eigenfunctions span the domain of the operator $L - ikc$ in Hilbert space.

4. Discussion

Conclusions (i)–(iii) at the end of §3 are the precise opposites of conclusions (i)–(iii) at the end of §2. The model operator L_1 of §3 is no less realistic than the model operator L_0 of §2, yet the two models lead to opposite results.

First, then, the conclusions of Foch and Ford (1970) concerning the normal mode solutions of the linearized Boltzmann equation are highly suspect. A model, no worse than theirs in its essentials, leads to precisely opposite results.

Second, the whole technique of working with mutilated model operators, rather than with the true Boltzmann equation, needs re-appraisal. Exact solutions of simple models constitute an exhilarating game for those who find this game exhilarating; but before the conclusions from such models can be used physically, it is necessary to give a physical discussion of the extent to which the model approximates the true physical situation. The two examples given here show that this physical discussion may have to be fairly intricate: In many respects L_0 and L_1 are physically similar; both have one zero eigenvalue, with the same eigenfunction, both are negative definite otherwise. Differences between them, likely to be relevant, are :

- (a) L_0 is bounded whereas L_1 is unbounded;
- (b) L_0 has an accumulation point in its spectrum, whereas L_1 has no accumulation point†;

† The author would like to thank the referee for pointing out the importance of accumulation points in the spectrum of the model operator L , and for the construction of formal arguments to this effect.

(c) L_1 is not only unbounded, but is 'more strongly unbounded' than the perturbation $-ikc$; that is, for large values of c the term $-4c^2$ in L_1 is larger than $-ikc$, no matter how big k is.

By making use of the formal expansion of an Hermitian operator in terms of its eigenvalues and eigenfunctions, and manipulating that expansion suitably, formal arguments can be constructed to suggest that at least some of these points (a), (b), and (c) are relevant to the final results (see footnote to previous page).

If these particular points are indeed relevant, then it follows that L_1 is a more realistic model operator than L_0 , or than any other bounded model operator. For Maxwell molecules, at least, the eigenfunctions and eigenvalues of the true L are known. The eigenfunctions are Burnett (three-dimensional linear harmonic oscillator) functions. The eigenvalues μ_{nl} are discrete, real, non-positive, and have no accumulation point. μ_{nl} tends to $-\infty$ as $n+l$ tends to infinity. It is interesting to observe, furthermore, that for the special case $l = 0$ the asymptotic behaviour of the eigenvalues is $\mu_{n0} \sim -An$ ($A = \text{constant}$), as shown in appendix C of Wang Chang and Uhlenbeck. This asymptotic behaviour is highly reminiscent of our simple model operator L_1 . For all these reasons, we suggest that not only is L_1 just as good a model as L_0 , but actually L_1 is a much better model.

We emphasize that all this is in the nature of surmise and conjecture. The truth can be found only from a careful study of the actual equations to be solved, not from guesses based on exact solutions of exceedingly simplified model equations.

In particular, it is an interesting question in pure mathematics to decide what are the conditions on a negative, unbounded operator L , with a discrete spectrum, to make L dominate over another unbounded operator X with a purely continuous spectrum; 'domination' here means that $L - ikX$ should have a purely discrete spectrum, for all real values of the parameter k .

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