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# A non-linear Boltzmann equation with analytic solutions

S Rouse and S Simons

Department of Applied Mathematics, Queen Mary College, Mile End Road, London E1 4NS, UK

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**Abstract.** An analytic solution is obtained for a certain non-linear one-dimensional Boltzmann equation describing the temporal relaxation to equilibrium of a system of particles, and its general features are elucidated. A solution is also found for the corresponding linearised problem and for two BGK models, one with the correct energy-dependent and the other with a mean energy-independent relaxation time. On comparing these with the solution of the non-linear equation, the main conclusions reached are that the accuracy of the linearised equation is superior to that of the models, even for large displacements from equilibrium, and that the gain in accuracy of the energy-dependent BGK model over the energy-independent one may well be offset by the additional computational work involved in using the former. Finally, a calculation of the successive time derivatives of the entropy, based on the exact non-linear equation, show that these alternate in sign, at least up to the tenth derivative.

## 1. Introduction

The main difficulties encountered in solving the non-linear Boltzmann equation are largely due to the complex mathematical nature of the collision term. The detailed form of this term depends on the precise nature of the intermolecular potential, but in all cases, the integrand of this term has two basic properties: (i) a particular type of non-linearity in the distribution function involved; and (ii) a mathematical form corresponding to the conservation of certain physical quantities (number, energy and momentum) in a collision. Krook and Wu (1976) were able to solve the equation for the case of a particular collision kernel and special boundary conditions, and Truesdell (1956) obtained an exact solution for a special shear flow problem. However, no analytic results have been obtained for the general time-dependent equation. It was therefore considered worthwhile to obtain an analytic solution to a problem, which while substantially simpler than the real problem, nevertheless embodies the above two basic properties of the true collision operator. The main simplification we employ is to consider a one-dimensional problem corresponding to the relaxation to equilibrium of a homogeneous molecular distribution initially in some arbitrary state. For this one-dimensional situation it is impossible to obtain a change in the number of molecules with a particular energy if both energy and momentum are conserved in collisions. We therefore dispense with conservation of momentum, and consider the situation where only number and energy are conserved. In order to define the problem uniquely it is necessary to specify the scattering kernel, and here we make the

obvious choice of taking a kernel which allows an analytic solution to be obtained. As we shall see in § 2, this property holds if the kernel is a constant, and our collision operator may thus be considered as corresponding to a one-dimensional analogue of Maxwell molecules. It should be noted that in order to utilise the mathematical approach of § 2, it is necessary to discretise the molecular energy states rather than allowing them to form a continuum. Finally we should mention that although the essential reasons for following our approach are those given above, one can nevertheless conceive of a real physical system described by the one-dimensional Boltzmann equation (3) that we shall employ. Consider an assembly of identical polyatomic molecules whose vibrational energy levels are quantised in integer multiples of an energy quantum,  $\epsilon$ . If an assembly of these molecules retains throughout a Maxwell equilibrium distribution in their velocities and if on collision they only exchange energy between their respective vibrational modes, then for a constant collision kernel our equation (3) will represent the decay to an equilibrium distribution of their vibrational energy states.

Apart from the intrinsic interest in deriving an analytic solution to a non-linear Boltzmann equation, the results we obtain are also of value in assessing the accuracy of certain simplified equations which have been traditionally employed. For a system close to equilibrium the linearised Boltzmann equation is known to be valid, but in general no estimate can be readily made of the errors arising when this equation is used for large departures from equilibrium. For such large departures model equations are often employed, the most popular being the BGK model†. This can be developed either with the correct velocity-dependent relaxation time or with an averaged (velocity-independent) relaxation time. In both cases, however, little is known about the error introduced by the use of the model. For the present non-linear collision operator we shall see that the linearised version and BGK models (with both velocity-dependent and velocity-independent relaxation times) may be readily formulated, and the consequent accuracies of three types of approximation may thus be estimated for different sets of initial conditions.

Finally, we have examined for the present non-linear system the sign of successive time derivatives of the entropy  $S$ . It is known that for several isolated systems these derivatives alternate in sign; that is,

$$(-1)^p d^p S/dt^p \leq 0 \quad (1)$$

where  $1 \leq p \leq M$ , and  $M$  may be finite or infinite (see Rouse and Simons 1976 for references to earlier work). Although the result (1) is known to hold for systems described by the linear Boltzmann equation with  $M = \infty$ , it has only been shown to be true for one very specialised non-linear case with  $M = 4$  (Rouse and Simons 1976). For our present one-dimensional system we have considered an initial situation drastically removed from equilibrium and have shown that the result (1) holds throughout the relaxation back to equilibrium with  $M = 10$ .

The nature of the mathematical approach we follow for the solution of the basic non-linear equation (3) has some points in common with that used by Kac (1956). The basic aims and treatment of his paper are, however, very different from ours.

† In this paper we have considered only the original BGK model because of its relative simplicity. At the expense of a substantially greater amount of work the approach used here could be applied to the more sophisticated models discussed by Cercignani (1969).

**2. The non-linear equation**

The non-linear Boltzmann equation for a spatially uniform gas relaxing to equilibrium can be expressed in the form

$$\frac{\partial f}{\partial t} = \iiint P(f_2 f_3 - f f_1) dv_1 dv_2 dv_3 \tag{2}$$

where  $f_p = f(\mathbf{v}_p)$  is the distribution function for molecules of velocity  $\mathbf{v}_p$  and  $P(\mathbf{v}, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$  is the interaction kernel. In accordance with the simplification given in the previous section, we proceed to consider the discrete one-dimensional analogue of equation (2) in which the energy of each molecule is given by  $n\epsilon$  where  $n$  is an integer ( $\geq 1$ ) and  $\epsilon$  is a unit of energy. The molecular state is considered to be specified by the energy alone, and so  $f \equiv f(n, t)$  gives the number of molecules with energy  $n\epsilon$  at time  $t$ . We suppose energy to be conserved in interactions, and assume  $P$  to be a constant, which we take as unity. The time-dependent Boltzmann equation then takes the form

$$\frac{\partial f(n)}{\partial t} = \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \sum_{n_3=1}^{\infty} (f(n_2)f(n_3) - f(n)f(n_1)) \tag{3}$$

where the sums are subject to the constraint  $n + n_1 = n_2 + n_3$ . Thus we obtain

$$\frac{\partial f(n)}{\partial t} = \sum_{\substack{n_2, n_3 \\ n_2+n_3>n}} f(n_2)f(n_3) - f(n) \sum_{n_1=1}^{\infty} (n + n_1 - 1)f(n_1). \tag{4}$$

Now the total number of molecules  $N$ , and their total energy  $E\epsilon$  remain constant throughout the temporal development of the system, and so we have

$$\sum_{n=1}^{\infty} f(n) = N \tag{5a}$$

$$\sum_{n=1}^{\infty} n f(n) = E. \tag{5b}$$

On making use of equations (5) we find that equation (4) can be expressed in the form

$$\frac{\partial f(n)}{\partial t} + [(n - 1)N + E]f(n) = N^2 - \sum_{\substack{n_2, n_3=1 \\ n_2+n_3 \leq n}} f(n_2)f(n_3). \tag{6}$$

This equation will yield a unique solution describing the relaxation of the system to equilibrium† if supplemented by boundary conditions of the form

$$f(n) = g(n) \quad \text{at } t = 0 \quad (1 \leq n \leq \infty). \tag{7}$$

Equation (6) can clearly be solved for successive values of  $n$ . Starting with  $n = 1$  the second term on the right-hand side is zero and so a solution for  $f(1, t)$  may be found. Substituting this into the right-hand side for  $n = 2$  allows a solution to be obtained for  $f(2, t)$  and so on for increasing values of  $n$ . We have, however, been able to obtain a

† An  $H$  theorem may be readily formulated for equation (3) in the same way as for equation (2), showing that as  $t \rightarrow \infty$ , the system must tend to an equilibrium state characterised by a Maxwell equilibrium distribution.

general solution of equation (6) of the form

$$f(n, t) = \sum_{u,v=0}^{u+v \leq n} C_{uv}^{(n)} \exp[-(uN + vE)t] \tag{8}$$

where  $C_{uv}^{(n)}$  is a constant (considered further below), and this we now proceed to prove. Assuming the form (8), we have

$$\begin{aligned} & \sum_{\substack{n_2+n_3 \leq n \\ n_2, n_3=1}} f(n_2)f(n_3) \\ &= \sum_{\substack{n_2+n_3 \leq n \\ n_2, n_3=1}} \sum_{\substack{u-s+v-w \leq n_2 \\ u-s, v-w=0}} \sum_{\substack{s+w \leq n_3 \\ s, w=0}} C_{u-s, v-w}^{(n_2)} C_{sw}^{(n_3)} \exp[-(uN + vE)t] \\ &= \sum_{u,v=0}^{u+v \leq n} \sum_{s=0}^u \sum_{w=0}^v \sum_{n_2=(u+v)-(s+w)}^{n-(s+w)} \sum_{n_3=s+w}^{n-n_2} C_{u-s, v-w}^{(n_2)} C_{sw}^{(n_3)} \exp[-(uN + vE)t] \tag{9} \end{aligned}$$

on changing the order of summations and defining  $C_{00}^{(0)} = 0$ . Substituting from equations (8) and (9) into (6) gives

$$\begin{aligned} & \sum_{u,v=0}^{u+v \leq n} [(n-u-1)N + (1-v)E] C_{uv}^{(n)} \exp[-(uN + vE)t] \\ &= N^2 - \sum_{u,v=0}^{u+v \leq n} \sum_{s=0}^u \sum_{w=0}^v \sum_{n_2=(u+v)-(s+w)}^{n-(s+w)} \sum_{n_3=s+w}^{n-n_2} C_{u-s, v-w}^{(n_2)} C_{sw}^{(n_3)} \exp[-(uN + vE)t] \end{aligned}$$

and by comparison of coefficients of  $\exp[-(uN + vE)t]$ , we obtain

$$C_{uv}^{(n)} = - \frac{\sum_{s=0}^u \sum_{w=0}^v \sum_{n_2=(u+v)-(s+w)}^{n-(s+w)} \sum_{n_3=s+w}^{n-n_2} C_{u-s, v-w}^{(n_2)} C_{sw}^{(n_3)}}{(n-u-1)N + (1-v)E} + \frac{N^2 \delta_{u0} \delta_{v0}}{(n-1)N + E} \tag{10a}$$

for  $u \neq n-1$  and  $v \neq 1$ .  $C_{n-1,1}^{(n)}$  remains as an arbitrary constant. The treatment leading to equation (10a) remains valid as long as  $(n-u-1)N + (1-v)E \neq 0$  for all  $u \neq n-1$  and  $v \neq 1$ . If, however,  $E/N$  is a rational fraction so that  $(n-u-1)N + (1-v)E = 0$  for some  $u = a$  and  $v = b$  with  $a \neq n-1$  and  $b \neq 1$ , then it may be shown that equation (8) still holds with  $C_{uv}^{(n)}$  given by equation (10a) for  $u \neq a, v \neq b$ , while  $C_{ab}^{(n)}$  takes the form

$$C_{ab}^{(n)} = -t \sum_{s=0}^a \sum_{w=0}^b \sum_{n_2=(a+b)-(s+w)}^{n-(s+w)} \sum_{n_3=s+w}^{n-n_2} C_{a-s, b-w}^{(n_2)} C_{sw}^{(n_3)}. \tag{10b}$$

It is clear that the above solution (8) combined with the recurrence relations (10) gives a unique result for  $f(n, t)$ , apart from the single arbitrary coefficient  $C_{n-1,1}^{(n)}$  which exists for each  $n$ . This coefficient may therefore be chosen to satisfy the boundary conditions (7). For specified  $g(n)$ , the general procedure is first to calculate  $N$  and  $E$  from equations (5), letting  $f(n) = g(n)$ . Taking  $n = 1$ , the set of coefficients  $C_{uv}^{(1)}$  are then readily obtained from equations (10) for  $(u, v) \neq (0, 1)$ , making use of  $C_{00}^{(0)} = 0$ . The boundary condition (7) applied to  $n = 1$  allows  $C_{01}^{(1)}$  to be obtained. The procedure is then repeated for successive values of  $n$ . It is clear that apart from the initial calculation of  $N$  and  $E$ , the solution thus obtained for  $f(n, t)$  is independent of  $g(m)$  for  $m > n$ .

Finally, we consider the form that  $f(n, t)$  takes as  $t \rightarrow \infty$ . It is clear from equation (8) that  $f(n, \infty) = C_{00}^{(n)}$  and the form for  $f(n, \infty)$  could thus be obtained from equations (10). A quicker way, however, is through the standard  $H$  theorem approach, by which

it is readily shown from equation (3) that, corresponding to conservation of number and energy, the Maxwell equilibrium distribution is given by

$$f(n, \infty) = \alpha\beta^{n-1} \tag{11a}$$

for constants  $\alpha$  and  $\beta$ . These two constants are in turn determined by equations (5) applied to  $f(n, \infty)$ ; these give

$$\alpha = N^2/E \quad \text{and} \quad \beta = 1 - (N/E). \tag{11b}$$

### 3. The linearised equation

We consider here the situation when  $f(n, t)$  is close to the equilibrium distribution  $f_0(n)$  ( $= f(n, \infty)$ ) as given by equation (11)). We let

$$f(n, t) = f_0(n)(1 + \phi(n, t)) \tag{12}$$

and substituting into equation (6), obtain

$$\frac{\partial \phi(n)}{\partial t} + [(n-1)N + E]\phi(n) = -\frac{2}{f_0(n)} \sum_{r,s=1}^{r+s \leq n} f_0(r)f_0(s)\phi(r). \tag{13}$$

Here we have neglected terms quadratic in  $\phi$  and have utilised the fact that  $f_0(n)$  satisfies equation (6) with  $\partial f/\partial t = 0$ . We proceed to show that a solution of equation (13) can be found of the form

$$\phi(n, t) = \sum_{r=0}^{n-1} D_r^{(n)} \exp[-(E + rN)t] \tag{14}$$

for constant  $D_r^{(n)}$ . On substituting from equation (14) into equation (13) and changing the order of summations, it is found that

$$\sum_{r=0}^{n-1} (n-r-1)ND_r^{(n)} \exp(-rNt) = 2N \sum_{r=0}^{n-2} \sum_{s=r+1}^{n-1} \left[ 1 - \left( 1 - \frac{N}{E} \right)^{s-n} \right] D_r^{(s)} \exp(-rNt).$$

Hence by comparison of the coefficients of  $\exp(-rNt)$  we obtain

$$D_r^{(n)} = \frac{-2}{n-r-1} \sum_{s=r+1}^{n-1} \left[ \left( 1 - \frac{N}{E} \right)^{s-n} - 1 \right] D_r^{(s)} \tag{15}$$

for  $0 \leq r \leq n-2$ , while  $D_{n-1}^{(n)}$  is arbitrary. A unique solution is obtained for  $\phi(n, t)$  if the Boltzmann equation is supplemented with boundary conditions of the form

$$\phi(n, 0) = \theta(n). \tag{16}$$

Starting with  $n = 1$ , the above discussion shows that  $D_0^{(1)}$  is arbitrary and may therefore be determined by equation (16) with  $n = 1$ . For successively higher values of  $n$ ,  $D_r^{(n)}$  is obtained from equation (15) for  $0 \leq r \leq n-2$ , while  $D_{n-1}^{(n)}$  is found from the relevant boundary condition (16). As in the non-linear case, it is clear that the form obtained for  $\phi(n, t)$  is independent of  $\theta(m)$  for  $m > n$ .

**4. The BGK model**

Following Simons (1972), we proceed to derive the BGK model corresponding to the collision operator in equation (3) by taking

$$\left(\frac{\partial f(n)}{\partial t}\right)_m = \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \sum_{n_3=1}^{\infty} (F(n_2)F(n_3) - f(n)F(n_1)) \tag{17}$$

where the sums are subject to the constraint  $n + n_1 = n_2 + n_3$ . Here  $F(n_p)$  ( $p = 1, 2, 3$ ) represents an equilibrium distribution of the form (11), characterised by as yet undetermined parameters  $N'$  and  $E'$ ; that is

$$F(n) = \frac{N'^2}{E'} \left(1 - \frac{N'}{E'}\right)^{n-1}, \tag{18}$$

where in general both  $N'$  and  $E'$  depend on  $t$ . The right-hand side of equation (17) will be zero if  $f(n) = F(n)$ , and so equation (17) may be expressed as

$$\left(\frac{\partial f(n)}{\partial t}\right)_m = \nu(F(n) - f(n)) \tag{19}$$

where

$$\nu = \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{n+n_1-1} F(n_1) = (n-1)N' + E'. \tag{20}$$

The parameters  $N'(t)$  and  $E'(t)$  are now determined by the conditions that the model (19) should overall conserve number and energy. This corresponds to

$$\sum_{n=1}^{\infty} \nu F(n) = \sum_{n=1}^{\infty} \nu f(n) \quad \text{and} \quad \sum_{n=1}^{\infty} n\nu F(n) = \sum_{n=1}^{\infty} n\nu f(n), \tag{21}$$

and substitution into these equations from equations (18) and (20) gives

$$NN' - N' + 2N'E' - N'E - E'N = 0 \tag{22a}$$

and

$$E'^2 - N'E' + EN' - EE' = N' \sum_{n=1}^{\infty} n^2(f(n) - F(n)). \tag{22b}$$

Equations (19) and (20), with  $N'$  and  $E'$  subject to the constraints (22) for all  $t$ , give the BGK model for the present situation.

A considerable simplification is achieved in the use of the BGK model if  $\nu$  can be taken as independent of  $n$ . For such a  $\nu$  it is seen from equations (21) and (5) that

$$N' = N \quad \text{and} \quad E' = E. \tag{23}$$

We can obtain a  $\nu$  of this form by averaging the above  $\nu$  (equation (20)) over all  $n$ , using  $f(n)$  as a weighting factor. That is, we take

$$\bar{\nu} = \frac{\sum_{n=1}^{\infty} [(n-1)N' + E']f(n)}{\sum_{n=1}^{\infty} f(n)} = 2E - N \tag{24}$$

from equations (5) and (23). It is clear that  $\bar{\nu}$  (unlike  $\nu$ ) is now independent of  $t$ , and the solution of equation (19) embodying the boundary conditions (7) can be explicitly

obtained in the form

$$f(n) = F(n) + (g(n) - F(n)) \exp[-(2E - N)t] \tag{25}$$

where now  $F(n) = f(n, \infty)$ , given by equation (11). It is clear that in this case  $f(n)$  is independent of  $g(m)$  for  $m \neq n$ .

Finally, it should be noted that in the last case the relaxation of  $f(n)$  to equilibrium is of necessity a monotonic variation, while in the three previous cases considered there exists the possibility of oscillatory behaviour in time.

### 5. Evaluation of the solutions

We proceed to apply the methods developed in the preceding three sections to three sets of initial conditions and in each case we consider the decay of  $f(n)$  to equilibrium for  $1 \leq n \leq 12$ . The sets of boundary conditions taken are (see equation (7))

$$\text{Condition A: } g(n) = \begin{cases} \text{constant} & (1 \leq n \leq 12) \\ 0 & (n > 12) \end{cases}$$

$$\text{Condition B: } \begin{aligned} g(n) &= 0 & (n \neq 5, 6) \\ g(6)/g(5) &= 1.33/0.67. \end{aligned}$$

This corresponds to placing the molecules initially in a narrow distribution well away from equilibrium. We occupy two states rather than one to avoid the anomalous situation leading to equation (10*b*), and we choose this occupied region to be fairly central in order to examine the variation in the ‘wings’ on both sides of the initially occupied states.

$$\text{Condition C: } g(n) \propto \left[ \frac{N_1^2}{E_1} \left(1 - \frac{N_1}{E_1}\right)^{n-1} + \frac{N_2^2}{E_2} \left(1 - \frac{N_2}{E_2}\right)^{n-1} \right]$$

with

$$N_1/E_1 = \frac{1}{18}, \quad N_2/E_2 = \frac{1}{2}, \quad N_1/N_2 = \frac{1}{3}.$$

This corresponds to a mixture of two very different equilibrium distributions.

For each set of boundary conditions we calculate the solution of:

(a) The exact non-linear equation as given by equations (8). The coefficients  $C_{uv}^{(n)}$  were first evaluated by computer from equations (10*a*) and the values of  $f(n, t)$  for various values of  $t$  were then computed from equation (8).

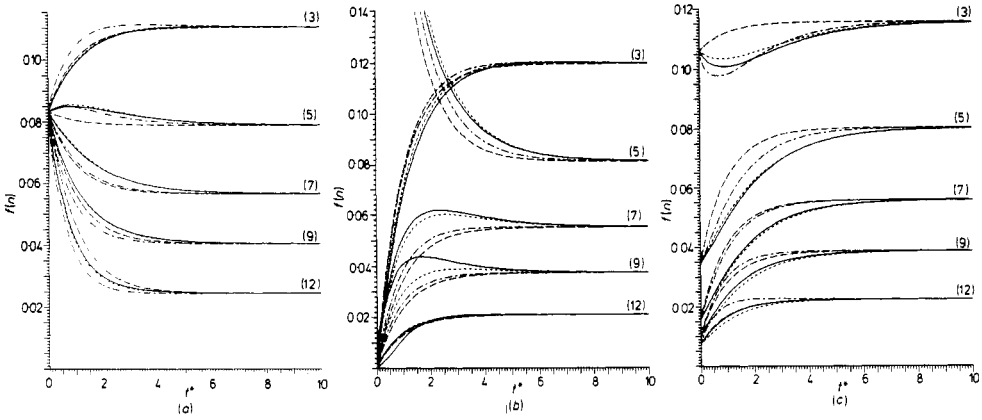
(b) The linearised equation as given by equation (14), for various values of  $t$ , using coefficients  $D_r^{(n)}$  computed from the recurrence relation (15).

(c) The ‘constant  $\nu$ ’ BGK model as given by equation (25) for various values of  $t$ .

(d) The ‘variable  $\nu$ ’ BGK model as given by the solution of equation (19) subject to the constraints (22). This case necessitated the use of a numerical integration technique outlined in the appendix.

The results of these computations are exhibited graphically in figure 1 and the graphs correspond respectively to the above boundary conditions A, B and C. In these graphs we take as abscissa a dimensionless time variable  $t^* = \bar{\nu}t$  with  $\bar{\nu}$  given by equation (24), and consider  $0 \leq t^* \leq 10$ . We determine the above boundary conditions





**Figure 1.**  $f(n, t^*)$  against  $t^*$  for various  $n$ . The figure in brackets is  $(n)$ . —, non-linear; ---, linear; — — —, 'constant  $\nu$ ' BGK model; - · - · -, 'variable  $\nu$ ' BGK model. (a), (b) and (c) correspond respectively to the three sets of initial conditions  $A, B$  and  $C$  specified in the text.

$A, B$  and  $C$  uniquely by the requirement that

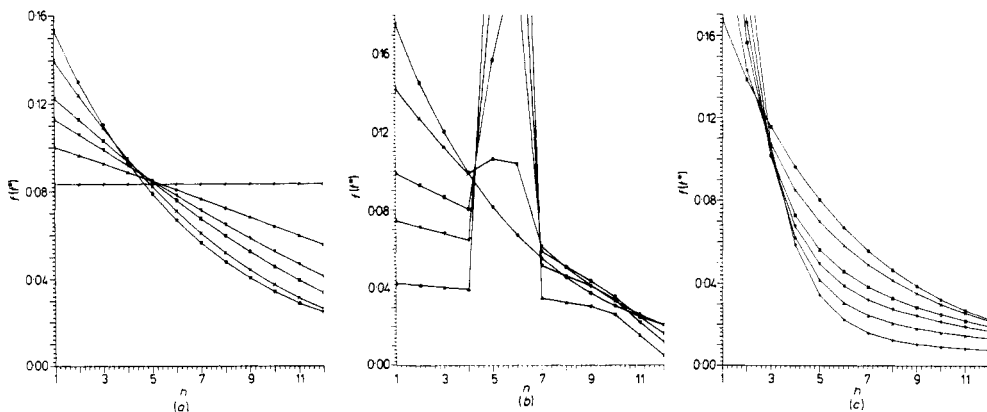
$$\sum_{n=1}^{\infty} g(n) = 1,$$

which is equivalent to  $N = 1$  (see equation (5a)), and the ordinate in each figure then gives the corresponding  $f(n, t^*)^\dagger$ . Values of  $n = 3, 5, 7, 9, 12$  are shown in each graph, and for each such value of  $n$  we depict the forms for  $f$  given by the solution of the four equations (a), (b), (c), (d) given above. In figure 2 we show  $f$  as a function of  $n$  for various values of  $t^*$  corresponding to the exact solution of the non-linear equation, and for the three sets of boundary conditions  $A, B$  and  $C$ .

We consider first the form of the exact solution of the non-linear equation as a function of time for various  $n$ . It is clear from figure 1 that in the majority of cases  $f(n, t^*)$  relaxes back monotonically from its initial value to its equilibrium value, but in some cases it passes through a maximum or minimum before attaining its final value. However, in no case has more than one such stationary value been found. The time for  $f(n, t^*)$  to effectively reach its equilibrium value varies to some extent with  $n$  and with the detailed boundary conditions, but is typically given by  $t^* \sim 5$ .

If we now compare the solution of the exact non-linear equation with the three approximations (b), (c) and (d) given above, perhaps the most surprising result is that in virtually all cases the solution of the linearised equation gives the best approximation, even when the condition  $|\phi| \ll 1$  (see equation (12)), which is usually assumed to be necessary for its validity, is not satisfied. As regards the two BGK approximations, it is clear that the 'constant  $\nu$ ' BGK model cannot be a good approximation when a stationary value exists in  $f(t^*)$  since, as mentioned earlier, this approximation must yield a monotonic return to equilibrium. This is borne out by figure 1 where the 'constant  $\nu$ ' BGK is always the worst approximation in cases where a stationary value

<sup>†</sup> If boundary conditions of the above form  $A, B$  and  $C$  are considered, but with  $\sum_{n=1}^{\infty} g(n) = \alpha$ , it is readily shown from equation (3) that the corresponding solution  $f_\alpha(n, t^*)$  is given by  $f_\alpha(n, t^*) = \alpha f(n, \alpha t^*)$ .



**Figure 2.**  $f(n, t^*)$  against  $n$  for various  $t^*$ .  $\diamond$ ,  $t^* = 0$ ;  $\triangle$ ,  $t^* = 0.5$ ;  $\nabla$ ,  $t^* = 1.0$ ;  $\square$ ,  $t^* = 1.5$ ;  $\times$ ,  $t^* = 3$ ;  $\circ$ ,  $t^* = 10$ .  $f(n, t^*)$  represents the solution of the non-linear equation for all curves. (a), (b) and (c) correspond respectively to the three sets of initial conditions A, B and C.

occurs. In other cases, however, comparison of the two BGK models shows that neither is consistently closer to the true result. In order, therefore, to make some kind of quantitative comparison of their relative accuracy, the following two quantities were calculated:

$$A(t^*) = \sum_{n=1}^{12} (f_{\nu}(n, t^*) - f(n, t^*))^2$$

$$B(t^*) = \sum_{n=1}^{12} (f_{\bar{\nu}}(n, t^*) - f(n, t^*))^2.$$

Here  $f$  is the solution of the exact non-linear problem, while  $f_{\nu}$  and  $f_{\bar{\nu}}$  are respectively the solutions for the ‘variable  $\nu$ ’ and ‘constant  $\nu$ ’ BGK models. The values of  $A(t^*)$  and  $B(t^*)$  were computed for  $1 \leq t^* \leq 10$ , for the three sets of boundary conditions and the results compared. In all cases it was found that  $A(t^*) < B(t^*)$  with  $A/B$  lying in the range 0.3–1.0 in virtually all cases. This suggests that on the whole the ‘variable  $\nu$ ’ model is better than the ‘constant  $\nu$ ’ model as indeed would be expected from the way in which they were derived. However the loss in accuracy in using the ‘constant  $\nu$ ’ model is not great and these inaccuracies may well be offset by the fact that the computations involved with the ‘constant  $\nu$ ’ model are considerably simpler than those arising with the ‘variable  $\nu$ ’ model. If these results remain true in a real three-dimensional interaction problem, they will tend to support the approach of the majority of workers in the field of kinetic theory, who have assumed a ‘constant  $\nu$ ’ BGK model without considering the errors introduced by neglecting the velocity dependence of  $\nu$ .

In view of the remarks at the beginning of the previous paragraph, it would clearly be of interest to compare the solutions of the non-linear and linearised problems in a real three-dimensional situation in order to examine whether the solution of the linearised problem is a reasonable approximation even when the system is far from equilibrium.

## 6. Entropy production

The standard definition of entropy  $S$  applied to our system gives

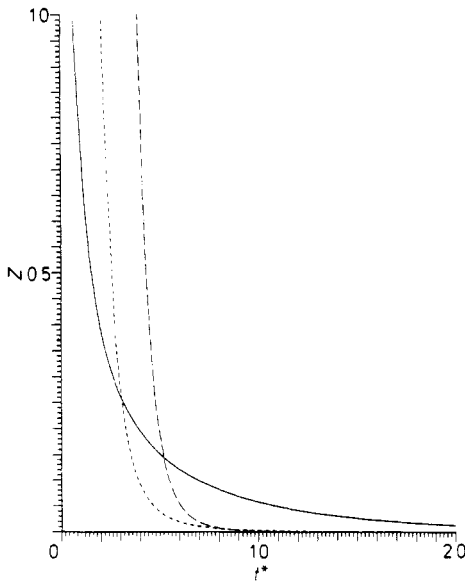
$$S = -k \sum_{n=1}^{\infty} f(n) \ln f(n), \quad (26)$$

and according to the discussion in the introduction, we are interested in examining the sign of successive time derivatives of  $S$ . By direct differentiation of equation (26) expressions for  $d^p S/dt^p$  can be obtained in terms of  $d^m f/dt^m$  ( $1 \leq m \leq p$ ), but these expressions become rapidly more complicated as  $p$  increases. In view of this it was decided to consider the range  $1 \leq p \leq 10$  for which the sign of  $S^{(p)}$  ( $= d^p S/dt^p$ ) can be obtained by plotting graphs of  $S^{(p)}$  as a function of  $t^*$  for  $p = 2, 5, 8$ .

In order to define the situation uniquely it is necessary to specify  $g(n)$ —the value of  $f(n)$  at  $t^* = 0$ . Various considerations motivate the choice for this, and we now proceed to consider these. Since it is known that the alternating hypothesis (1) holds when the linearised equation is valid close to equilibrium (Simons 1971), it is clear that to subject this hypothesis to a stiff test the initial distribution should be well away from equilibrium. We therefore put the majority of the molecules into two states which are chosen to correspond to  $n = 2$  and 3 in order to minimise the contribution to  $S^{(p)}$  of states with  $n > 12$ , for which it cannot be computed. However we cannot leave all other states completely unoccupied since this would lead to  $S^{(p)}$  becoming infinite at  $t = 0$  due to factors of  $f(n)$  in the denominator of the expression for  $S^{(p)}$ . Since we also wish to minimise the contribution to  $S^{(p)}$  arising from states with  $n > 12$ , it seems reasonable to take for  $n > 12$ ,  $g(n)$  equal to the final equilibrium value of  $f(n)$  at  $t^* = \infty$ , as this should tend to minimise the changes in  $f(n)$  as  $t^*$  increases. In order to check that these changes are indeed small this 'equilibrium value' for  $g(n)$  was used for  $n \geq 9$  so that the variation in  $f(n)$  for  $9 \leq n \leq 12$  could be directly examined. To avoid  $S^{(p)}$  becoming infinite we take  $g(n) = 10^{-4}$  for  $n = 1, 4, 5, 6, 7, 8$  and having chosen  $N = 1$ ,  $E = 2.4$ ,  $g(n)$  is then specified uniquely for all  $n$ .

Using the above boundary conditions, the values of  $S^{(p)}(t^*)$  for  $p = 2, 5, 8$  were computed for  $0 \leq t^* \leq 2$ , the required values of  $d^m f(n, t^*)/dt^{*m}$  being obtained by direct differentiation of the exponential function in equation (8). As explained above, the sums over  $n$  arising from equation (26) with range  $1-\infty$  were replaced by range  $1-12$  and the contributions to these sums from  $n = 9, 10, 11, 12$  were separately calculated. Figure 3 shows the resulting graphs of  $-S^{(2)}/k$ ,  $S^{(5)}/k$  and  $-S^{(8)}/k$  for  $t^* \leq 2$ . The decrease in value of each of these functions at  $t^* = 2$  compared with its value at  $t^* = 0$  suggests that computation beyond  $t^* = 2$  is unnecessary. This is borne out by the closeness of the graphs in figure 1 for the non-linear and linear cases for  $t^* > 2$ . In all cases it was found that the contribution to  $S^{(p)}$  arising from  $n = 12$  was less than 2% of the total, and one might reasonably suppose that we are therefore justified in neglecting the contributions from larger values of  $n$  as these would be expected to become smaller as  $n$  increases, due to the particular state becoming progressively more immersed in equilibrium surroundings. This is supported by the smoothness of the graphs which would not have occurred if a substantial proportion of  $S^{(p)}$ , randomly varying, had been neglected.

Considering now the functions shown in the graphs of figure 3, it is clear that each is non-negative while its first and second derivatives are respectively non-positive and non-negative. The truth of equation (1) for the present situation has thus been demonstrated for  $1 \leq p \leq 10$ . Finally it should be noted that the extremely large (but



**Figure 3.**  $Z$  against  $t^*$ . —,  $Z = -10^{-2}S^{(2)}/k$ ; ----,  $Z = 10^{-5}S^{(5)}/k$ ; - · -,  $Z = -10^{-10}S^{(8)}/k$ .

finite) values of the given functions for very small  $t^*$  prevent them being shown in the above figure, but analysis of the numerical data shows that the above conclusion of the validity of equation (1) holds for values of  $t^*$  down to zero.

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**Appendix**

We consider here the solution of equation (19), with  $F(n, t)$  and  $\nu(n, t)$  given respectively by equations (18) and (20), subject to the constraints (22) which effectively define  $N'(t)$  and  $E'(t)$ . The complex nature of these constraints prevents the use of an analytic approach, and we therefore employ a numerical technique based on the result

$$f(n, t + \delta t) = (f(n, t) - F(n, t)) \exp(-\nu(n, t)\delta t) + F(n, t) \tag{A.1}$$

which follows from equation (19). Starting with  $t = 0$ ,  $f(n, t)$  was calculated from equation (A.1) for successive increases of  $\delta t$  in  $t$ . At each stage  $E'$  and  $N'$  were obtained numerically from the simultaneous solution of equations (22), and these values were then used in the next stage to specify  $F(n)$  and  $\nu$  from equations (18) and (20). In the solution of equations (22), the infinite upper limit in the sum on the right-hand side of equation (22b) was approximated by an integer  $I$ . The values of  $I$  and  $\delta t$  were then independently doubled and halved respectively until the corresponding change in  $f(n, t)$  was less than 1% for all  $n$  and  $t$ .

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