Numerical aspects of the approach to a Maxwellian distribution

John Tjon and Tai Tsun Wu*

Instituut voor Theoretische Fysica der Rijksuniversiteit, Utrecht, The Netherlands (Received 13 September 1978)

It has been conjectured, for the Boltzmann equation, that an arbitrary initial state tends first to relax towards a state characterized by the similarity solution. We present here a simple model where the possible validity of the statement can be studied numerically. The results of extensive numerical computation for the first time give support for the validity of this conjecture.

I. INTRODUCTION

Several years ago, Krook and Wu¹ analyzed the formation of Maxwellian tails, in the context of the Boltzmann equation for homogeneous isotropic distributions. The motivation was to study quantitatively certain gas-phase reactions. An especially important example is the controlled thermonuclear fusion of a confined hydrogen plasma. The taming of thermonuclear fusion is at present perhaps the most important technological challenge.

The results of the previous analysis¹ consist of an exact solution in one case and an asymptotic solution in another. The exact solution was also found by Bobylev.² Although special solutions are of interest in themselves, their importance is due to the possible special role played by similarity solutions. More explicitly, the conjecture is as follows.³ "An arbitrary initial state tends first to relax towards a state characterized by the similarity solution. The subsequent stages of the relaxation is essentially represented by the similarity solution with appropriate phase."

Although this conjecture can perhaps be considered to be reasonable on physical grounds, no evidence for or against this conjecture is known in the context of the Boltzmann equation. It is the purpose of this paper to initiate a numerical study of the possible validity of the above conjecture.

Because the nonlinear Boltmann equation is notoriously complicated, not much is known about it even a century after its inception. We have recently learned in a hard way that it is also very difficult to study numerically. Our main difficulty stems from the fact that the tail of the Maxwellian distribution, although of great importance physically, is numerically small. Numerically, analysis of the previous case¹⁻³ has not been accomplished, and instead we look for a simpler model. In Sec. II we describe this model in some detail and in Sec. III we give a physical interpretation that is not completely satisfactory. Even this simplified model is very difficult to program on a computer, and we thus formulate in Sec. IV a discrete version with all the necessary conservation laws. This discrete version is analyzed numerically in Sec. V, and the results given in Sec. VI.

The results indicate that the conjecture may indeed be true. However, it has to be remembered that, in addition to the inherent limitations of numerical analysis, we have also introduced modifications of the model and its discretization. Nevertheless, there is perhaps enough evidence now to encourage efforts to prove the conjecture at least for some simple circumstances.

II. MODEL

The collision term in the Boltzmann equation contains in general multidimensional integrations over the distribution function f. Confining ourselves to the spatial homogeneous case, we have

$$\frac{\partial f(\vec{\mathbf{v}},t)}{\partial t} + \int \left[f(\vec{\mathbf{v}},t) f(\vec{\mathbf{w}},t) - f(\vec{\mathbf{v}}',t) f(\vec{\mathbf{w}}',t) \right] \\ \times A \, d\vec{\mathbf{v}}' \, d\vec{\mathbf{w}}' \, d\vec{\mathbf{w}} = 0 \tag{2.1}$$

where the third term represents the contribution from collisions of particles with initial velocities \overline{v}' and \overline{w}' to particles with final velocities \overline{v} and \overline{w} . The collision matrix A is such that the normalization

$$N(t) = \int f(\mathbf{\bar{\nabla}}, t) \, d\mathbf{\bar{\nabla}} \tag{2.2}$$

and average energy

$$E(t) = \frac{1}{2} \int v^2 f(\vec{\mathbf{v}}, t) \, d\,\vec{\mathbf{v}}$$
(2.3)

are conserved quantities. In a previous paper an isotropic model for A was studied. The resulting Boltzmann equation in appropriately chosen units of time and velocity has the form

$$\frac{\partial f(v,t)}{\partial \tau} + f(v,\tau) - \frac{1}{4\pi} \int f(v',\tau) f(w',\tau) \\ \times \sin\chi \, d\chi \, d\epsilon \, d\vec{w} = 0, \qquad (2.4)$$

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where χ and ϵ are angles characterizing the twobody scattering process.

Since our main objective is to examine how the tail of the distribution function reaches equilibrium for various initial conditions, the study of an equation like (2.4) is very difficult in view of the complicated kernel. Instead we look for a simpler equation that is both physically meaningful and numerically tractable. Our starting point is the generating function for normalized moments

$$G(\xi, \tau) = \sum_{n=0}^{\infty} \xi^{n} M_{n}(\tau) , \qquad (2.5)$$

where the normalized moments are given by

$$M_{n}(\tau) = 4\pi \frac{2^{n} n!}{(2n+1)!} \int_{0}^{\infty} f(v,\tau) v^{2n+2} dv . \qquad (2.6)$$

This generating function G satisfies the nonlinear partial differential equation^{1,3}

$$\frac{\partial^2}{\partial\xi\partial\tau}\,\xi G + \frac{\partial}{\partial\xi}\,\xi G = G^2\,. \tag{2.7}$$

The relation between f and G is somewhat complicated. The substitution of (2.6) into (2.5) gives

$$G(\xi,\tau) = 4\pi \int_0^\infty dv \, K(\xi,v) f(v,\tau) \,, \qquad (2.8)$$

where

$$K(\xi, v) = v^{2} \sum_{n=0}^{\infty} \frac{2^{n} n!}{(2n+1)!} (\xi v^{2})^{n}$$
$$= \left(\frac{\pi}{2}\right)^{1/2} \xi^{-1/2} v \exp(\frac{1}{2}\xi v^{2}) \operatorname{erf}(\xi^{1/2} v),$$
(2.9)

with

$$\operatorname{erf}(x) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^x dx' \exp(-\frac{1}{2}x'^2).$$
 (2.10)

The model that we shall study in this paper is obtained by replacing the product of $\xi^{-1/2}$ with the error function by a constant. Define a new distribution function \overline{f} by

$$G(\xi,\tau) = \int_0^\infty v \, dv \exp(\frac{1}{2}\xi v^2) \overline{f}(v,\tau) \,. \tag{2.11}$$

We wish to find out how $\overline{f}(v,\tau)$ approaches the Maxwellian distribution as $\tau \to \infty$.

Is it justified to call \overline{f} a distribution function? We claim that it does have the basic properties of a distribution function in two dimensions. First, since¹

$$G(\xi,\tau) = 1 + \xi + O(\xi^2)$$
 (2.12)

as $\xi \to 0$ for all τ , we get, for all τ ,

$$\int_{0}^{\infty} v \, dv \overline{f}(v,\tau) = 1 \tag{2.13}$$

and

$$\frac{1}{2}\int_0^\infty v^3 dv \overline{f}(v,\tau) = 1. \qquad (2.14)$$

Thus the particle number and average energy are conserved and properly normalized. Second, as $\tau \rightarrow \infty$,

$$G(\xi, \tau) \to (1-\xi)^{-1},$$
 (2.15)

we get from (2.11) that

$$\overline{f}(v,\tau) \to \exp(-\frac{1}{2}v^2), \qquad (2.16)$$

which is precisely the Maxwellian distribution. We shall return to a more detailed interpretation of \overline{f} in Sec. III.

It is clearly desirable to use the variable

$$x = \frac{1}{2}v^2$$
. (2.17)

In terms of x, G, and \overline{f} are related by

$$G(\xi,\tau) = \int_0^\infty dx \, e^{x\xi} F(x,\tau) \,, \qquad (2.18)$$

where

$$F(x,\tau) = \overline{f}(v,\tau) . \qquad (2.19)$$

By (2.13), (2.14), and (2.16), F has the properties

$$\int_0^{\infty} F(x,\tau) \, dx = \int_0^{\infty} x \, F(x,\tau) \, dx = 1 \tag{2.20}$$

for all τ , and

$$F(x,\tau) \to e^{-x} \tag{2.21}$$

as $\tau \to \infty$.

With (2.20), the substitution of (2.18) into (2.17) gives the integrodifferential equation for $F(x, \tau)$:

$$\frac{\partial}{\partial \tau} F(x,\tau) + F(x,\tau) = \int_{x}^{\infty} dx' x'^{-1} \int_{0}^{x'} dx'' F(x'-x'',\tau) F(x'',\tau) .$$
(2.22)

This is the basic equation for the model to be studied.

III. PHYSICAL INTERPRETATION

In Sec. II we have derived, starting from the generating function $G(\xi, \tau)$, the corresponding Boltzmann equation for the distribution function, its Laplace transform being $G(\xi, \tau)$. We now turn to describe a model for the collision matrix A in the Boltzmann equation (2.1) which gives rise to the same equation if we confine ourselves to two dimensions. Let us consider a d-dimensional system in which the scattering between two parti-

cles takes place diffusively, but still satisfying energy conservation. The collision matrix A in (2.1) is assumed to be of the form

$$A = a\delta(v^2 + w^2 - v'^2 - w'^2), \qquad (3.1)$$

where a depends only on the total energy of the colliding particles and is taken to be

$$a = a_0 / (v^2 + w^2)^{d-1}.$$
(3.2)

Using (3.1) the Boltzmann equation for an isotropic distribution can be written

$$\frac{\partial f(v,\tau)}{\partial \tau} + f(v,\tau) - \int_0^\infty w^{d-1} dw \int_0^\infty v'^{d-1} dv'$$
$$\times \int_0^\infty w'^{d-1} dw' f(v',\tau) f(w',\tau)$$
$$\times a\delta(v^2 + w^2 - v'^2 - w'^2) = 0. \quad (3.3)$$

In order to have the normalization

$$N(\tau) = \int_0^\infty v^{d-1} dv f(v,\tau)$$
(3.4)

to be conserved and equal one, it is necessary to have

$$a_0 = 4\Gamma(d) / \Gamma(\frac{1}{2}d)^2$$
. (3.5)

It is readily verified that with the choice of a_0 we also have conservation of the average energy

$$E(\tau) = \frac{1}{2} \int_0^\infty v^{d+1} dv f(v, \tau) \,. \tag{3.6}$$

In this model clearly total momentum conservation is absent. A similar model has been considered in one dimension by Kac.⁴ It is felt that this nonconservation will not change qualitatively the results we have found. In particular, various models have been studied like the Lorentz system⁵⁻⁹ and the Ehrenfest wind-tree model, ¹⁰⁻¹² in which momentum conservation is violated while the nonequilibrium properties behave qualitatively in the same way as in the momentum-conserving cases. Furthermore, the Boltzmann *H* theorem holds for (3.3). The reason is that only energy conservation, not momentum conservation, is needed for the proof of the Boltzmann *H* theorem.

Introducing polar coordinates in the v', w' plane the Boltzmann equation (3.3) can be rewritten

$$\frac{\partial f(v,\tau)}{\partial \tau} + f(v,\tau)$$

$$= \frac{\Gamma(d)}{2^{d-2}\Gamma(d/2)^2} \int_0^\infty w^{d-1} dw$$

$$\times \int_0^{\tau/2} d\theta (\sin 2\theta)^{d-1} f[(v^2 + w^2)^{1/2} \sin \theta, \tau]$$

$$\times f[(v^2 + w^2)^{1/2} \cos \theta, \tau]. \qquad (3.7)$$

In contrast to the general case, the kernel of Eq. (3.7) is of a simpler form. In particular, if we consider the case d=2, (3.7) can be reduced to (2.22). By (2.17) and (2.19) (3.7) with d=2 can be rewritten

$$\frac{\partial F(x,\tau)}{\partial \tau} + F(x,\tau)$$

$$= \int_{0}^{\infty} dx' \int_{0}^{\tau/2} \sin 2\theta \, d\theta \, F[(x+x')\cos^{2}\theta,\tau]$$

$$\times F[(x+x')\sin^{2}\theta,\tau] \qquad (3.8)$$

or

$$\frac{\partial F(x,\tau)}{\partial \tau} + F(x,\tau)$$

$$= \int_0^\infty \frac{dx'}{x+x'} \int_0^{x+x'} dx'' F(x+x'-x'',\tau)F(x'',\tau),$$
(3.9)

which is precisely Eq. (2.2). Hence the basis equations we study correspond to the Boltzmann equation in two dimensions with diffusive scatter-ing between the particles.

IV. DISCRETE VERSION

Equation (2.22) is a nonlinear integrodifferential equation. It is simpler than the Boltzmann equation because the integral is a repeated integral, not a general double integral.

In order to solve this integrodifferential equation numerically, the continuous variable x is replaced by a discrete one, say $j \Delta$, where j = 0, 1, 2,3,... If, for example, Gaussian integration method is used, then it is necessary to interpolate between the various values of j. Interpolation can be avoided completely if the trapezoidal rule is used:

$$\int_0^{j\Delta} F(x) \, dx \to \sum_{i=0}^j e_i \epsilon_{j-i} F_i \, \Delta \,, \qquad (4.1)$$

where

$$F_j = F(j\Delta), \qquad (4.2)$$

and

$$\epsilon_j = \begin{cases} \frac{1}{2} & \text{for } j = 0, \\ 1 & \text{otherwise.} \end{cases}$$
(4.3)

Equation (4.1) holds for j > 0. If j = 0, it takes the peculiar form

$$\int_{0}^{0} F(x) \, dx \to \frac{1}{4} F_{0} \, \Delta \,. \tag{4.4}$$

We apply the trapezoidal rule to (2.22):

$$\frac{\partial F_i}{\partial \tau} + F_i - \Delta \sum_{k=i}^{\infty} \epsilon_{k-i} \frac{1}{k} \sum_{j=0}^{k} \epsilon_j \epsilon_{k-j} F_j F_{k-j} = 0. \quad (4.5)$$

Although (4.5) is thus obtained as an approximation to (2.22), it can be considered to be a model in its own right. So far as the physical interpretation of Sec. III is concerned, the only modification is that the possible energies are discrete. The only conditions on this discrete model is that the normalization and energy

$$N(\tau) = \Delta \sum_{j=0}^{\infty} \epsilon_j F_j$$
(4.6)

and

$$E(\tau) = \Delta^2 \sum_{j=0} jF_j$$
 (4.7)

are time independent.

Summation of (4.5) over *i* gives

$$\frac{dN(\tau)}{d\tau} + N(\tau) = \Delta^2 \sum_{i=0}^{\infty} \epsilon_i \sum_{k=i}^{\infty} k^{-1} \epsilon_{k-i} \sum_{j=0}^{k} \epsilon_j \epsilon_{k-j} f_j f_{k-j}$$
$$= \Delta^2 \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} \sum_{i=0}^{j+1} \epsilon_j \epsilon_l f_j f_l (j+l)^{-1} \epsilon_i \epsilon_{j+l-i}$$
$$= N(\tau)^2 .$$
(4.8)

Therefore $N(\tau_0) = 1$ at some τ_0 implies that

 $N(\tau) = 1 \tag{4.9}$

for all τ .

Similarly

$$\frac{dE(\tau)}{d\tau} + E(\tau) = \Delta^3 \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} \sum_{i=0}^{j+l} \epsilon_j \epsilon_l f_l (j+l)^{-1} i \epsilon_{j+l-i}$$
$$= N(\tau) E(\tau) .$$
(4.10)

Equations (4.9) and (4.10) imply that $E(\tau)$ is independent of τ .

V. NUMERICAL ANALYSIS

Equation (4.5) is solved numerically on a Cyber 73/28. In this numerical solution, a discrete time interval $\Delta \tau$ and an upper cutoff N in the number of points are used. In other words for $i=0, 1, 2, \ldots, N-1$ we calculate F_i at a later time $\tau + \Delta \tau$

$$F_{i}(\tau + \Delta \tau) = F_{i}(\tau)(1 - \Delta \tau) + \Delta \tau \Delta \sum_{k=i}^{N-1} \epsilon_{k-i} k^{-1}$$
$$\times \sum_{j=0}^{k} \epsilon_{j} \epsilon_{k-j} F_{j}(\tau) F_{k-j}(\tau) .$$

In order to get stable results with respect to the time integration it is necessary to renormalize F_i so that $N(\tau) = 1$ after each application of (5.1). Having obtained the solution in this way, a least-squares fit to the special solution of the continuum version of the model is carried out. More precisely, for each τ , the phase τ_0 is determined by

minimizing

$$\sum_{i=0}^{N_f-1} \left| F_i(\tau) - F_i^{(0)}(\tau - \tau_0) \right|^2.$$
(5.2)

We have not succeeded in finding exact special solutions of the discrete version of the model. However, since Δ has been chosen sufficiently small, we take in analogy to the special solution of the continuum model¹⁻³ for $F_n^{(0)}$

$$F_n^{(0)} = \gamma^n (A + nB),$$
 (5.3)

where γ , A, and B are functions of $\tau - \tau_0$. The coefficients A and B can be expressed in terms of γ using the conditions that (4.6) and (4.7) are to be equal to one. We find

$$A = 2(1 - \gamma)(1 + \gamma^2)^{-1}[(1 + \gamma)\Delta + (1 - \gamma)]/\Delta^2, \quad (5.4)$$

$$B = (1 - \gamma)^2 \gamma^{-1} (1 + \gamma^2)^{-1} [-2\gamma \Delta + (1 - \gamma^2)] / \Delta^2 . \quad (5.5)$$

Furthermore, γ can be parametrized as

$$\tau - \tau_0 = 6 \ln \left(1 + \frac{\Delta}{\ln(\gamma_{\infty}/\gamma)} \right)$$
 (5.6)

with

$$\gamma_{\infty} = -\Delta + (1 + \Delta^2)^{1/2} \,. \tag{5.7}$$

Although (5.3) is not an exact solution to the discrete model, we notice that the stationary solution can be determined exactly. It is given by

$$F_n^{(\infty)} = c \gamma_\infty^n \,. \tag{5.8}$$

Tests were carried out in how far the fits were sensitive to Δ and we have indeed found that the results for τ_0 were stable for variations of Δ . In addition to Δ , there are thus three parameters: $\Delta \tau$, N, and N_f.

In principle, the conjecture of Sec. I means that $\lim_{\tau \to \infty} \tau_0$ exists. However, this can be true only if N is infinite. Because of the finite N, we can at best get a τ_0 approximately independent of τ over a finite range of τ .

As a test of the dependence on $\Delta \tau$, and N_f , we first study in some detail the case where

$$F_n(0) = F_n^{(0)}(2)$$
 (5.8)

The result of the test is shown in Fig. 1, where $\Delta = \frac{32}{127}$. When $\Delta \tau = 0.1$ and N = 128, deviation from $\tau_0 = -2$ occurs later for smaller N_f . We thus conclude that for N = 128, a suitable choice for N_f is 74. To have some idea of the origin of the rapid deviation, we used a larger value of N = 192 with $N_f = 111$. The range of reasonably accurate τ_0 is found to be greatly extended. Thus the deviation from $\tau_0 = -2$ is due to the boundary effect of finite N. More accurate values of τ_0 can be obtained with smaller values of $\Delta \tau$.

We conclude from this test that the program is useful in giving indications of the possible validity



FIG. 1. Least-squares-fitted τ_0 as a function of time τ in the case that the initial distribution is taken to be the special solution for various choices of N, N_f , and $\Delta \tau$.

of the conjecture. A similar test with

 $F_n(0) = F_n^{(0)}(6) \tag{5.9}$

gives the same conclusion.

VI. NUMERICAL RESULTS

The numerical code has been used to study a number of initial conditions. In all cases, $\Delta = \frac{32}{127}$, N = 128, $N_f = 74$ are used, in some cases, other parameters are also used. In addition to the test cases (5.8) and (5.9), the other initial conditions are

(A) Maxwellian distribution with tail cutoff;

(B) A simple peak with $F_n(0) = 0$ except n = 3 and 4;

(C1) $F_n(0) = 0$ except n = 0 and 2;

(C2) $F_n(0) = 0$ except n = 0 and 4;

(C3) $F_n(0) = 0$ except n = 0 and 6;

(C4)
$$F_n(0) = 0$$
 except $n = 0$ and 7; and

(C5) $F_n(0) = 0$ except n = 0 and 8.

Note that (C1) is anomalous because in this case $F_0(0)$ is negative. We describe in this section some of the numerical results, with emphasis on the function $\tau_0(\tau)$. The least-squares fit to determine. τ_0 gives a very good fit in all cases except for small values of τ .

For case (A), τ_0 is virtually independent of τ , indicating that the conjecture applies well in this case. We therefore concentrate on initial condition that are more peaked and hence less similar to the special solution or the maxwellian distribution. It is on the basis of this criticism that the other cases are chosen. In Fig. 2, we show for case (B) the same plot as for the case (4.8). There is no qualitative and very little quantitative difference between Fig. 1 and Fig. 2, even though the initial conditions are quite different.

We next turn our attention to case (C). Consider first case (C2), where $F_4(0) \gg F_0(0)$. To get an



FIG. 2. Same as in Fig. 1 but the initial distribution is given by $F_n = 0$ except for n = 3, 4.

idea about the approach to Maxwellian distribution, we plot in Figs. 3 and 4 the normalized distribution function $F_n(\tau)/F_n^{(\infty)}$, where

$$F_n^{(\infty)} = [(1 - \gamma_\infty)\Delta]^2 \gamma_\infty^{n-1} \tag{6.1}$$

is the distribution function for $\tau \to \infty$ and $N \to \infty$. Figure 3 shows clearly the nonuniform approach to equilibrium of the distribution function where the higher velocity particles take longer times to reach equilibrium. From Fig. 4 we see that the relative changes in time of F_n for a fixed *n* are much larger in the initial times than when F_n is close to its stationary value. This is in accordance with the findings of Bobylev.² The decay time when F_n is near equilibrium is of the order of three which is consistent with the slowest decay time found for the moments.³ The effect of finite N is also clearly seen in Fig. 4, since $F_n(\tau)/F_n^{(\infty)}$ fails to reach 1 for n = 125. For both case (B) and case (C) below, $\Delta \tau = 0.025$ is used.

In Fig. 5 we plot $\tau_0(\tau)$ for all five cases of (C). For (C1) and (C2), τ_0 is nearly independent of τ for $\tau \leq 45$. For (C3), there is also some variation for small τ , indicating a rather rapid approach to



FIG. 3. Normalized distribution $F_n/F_n^{(\infty)}$ as a function of *n* for various τ . The initial distribution is given by $F_n = 0$ except for n = 0, 4. The parameters are N = 128, $\Delta \tau = 0.025$. The plot on the right shows a blow up view of the double peak near n = 5 for $\tau = 3$ and 5.

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FIG. 4. Normalized distribution $F_n/F_n^{(\infty)}$ as a function of τ for various *n*. The initial distribution is the same as in Fig. 3.

Maxwellian distribution for the reason originally studied by Maxwell. This effect at small τ becomes much more important for case (C4), and is completely dominating for case (C5). Indeed, for case (C5), there is no region of constant τ_0 at all. To see that this does not mean a failure of the conjecture, the computation is repeated for (C4) and (C5) with N=192. A region of nearly constant τ_0 then becomes evident.

Although already seen in Fig. 1 and 2; it is especially evident from Fig. 5 why for large τ the values of τ_0 fail to remain constant but increase rapidly. For given N, as $\tau \rightarrow \infty F_n(\tau)$ approaches a limit, say $F_n(\infty)$. These limiting values $F_n(\infty)$ are determined by (5.1) with $F_n(\tau + \Delta \tau) = F_n(\tau)$, and hence are independent of the initial conditions. Using the least-squares fit (5.2) by minimizing



FIG. 5. Least-squares-fitted τ_0 as a function of τ with the initial distribution $F_n = 0$ except for n = 0, m, for various choices of m. The parameters are N=128, N_f = 74, $\Delta \tau = 0.025$ for the solid curves and N=192, $N_f=74$, $\Delta \tau = 0.025$ for the dashed curves.

$$\sum_{i=0}^{N_f-1} \left| F_n(\infty) - F_n^{(0)}(\tau_{\infty}) \right|^2$$
(6.2)

determines τ_{∞} , which depends on Δ , N, and N_f, but not the initial conditions. In other words, for large τ ,

$$\tau_0 \sim \tau - \tau_\infty, \qquad (6.3)$$

representing the linear rise of $\tau_{\rm o},$ as seen in Figs. 1, 2, and 5.

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