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# THE PSEUDO-SHOCK : A NON-LINEAR PROBLEM OF TRANSLATIONAL RELAXATION

B. L. Hicks

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THE PSEUDO-SHOCK: A NON-LINEAR PROBLEM OF TRANSLATIONAL RELAXATION

B. L. Hicks

Abstract

The Boltzmann equation has been solved by Nordsieck's Monte Carlo method for the case of translational relaxation of a gas of elastic spheres whose initial velocity distribution function has the form

$$f(\vec{v},0) = \frac{1}{2}\left\{\exp[-\pi(\vec{v}-\vec{i}u)^2] + \exp[-\pi(\vec{v}+\vec{i}u)^2]\right\} .$$

The Mach number

$$M = (6\pi/5)^{\frac{1}{2}}u$$

describes the relative separation of the two peaks of the bimodal distribution function and therefore controls the degree of initial departure from equilibrium. Calculations have been made for M = 0.5, 1, 2, 4, and 6, which includes a range of initial conditions from very close to very far from thermal equilibrium.

In the early part of the translational relaxation we find that relaxation by a factor of $e^{-1}$ requires, on the average, 1.27 $\pm$ 0.044 collisions for the lateral temperature and 0.80 $\pm$ 0.033 collisions for the Boltzmann function H. The temperature relaxation rate is thus smaller by a factor of 1.58 $\pm$ 0.120 than the entropy relaxation rate. (The uncertainties are stated as 90% confidence limits.) These collision numbers are essentially independent of M and time, at least until each molecule has made about ten collisions. Our calculations agree with earlier, more qualitative results in the literature that

correspond to different initial conditions. We have also shown that in a Krook model of our relaxation process, the ratio of the two collision numbers is somewhat smaller than two late in the relaxation and, as shown also by Offerhaus, approaches two asymptotically.

Solution of the Boltzmann equation for any other reasonable initial conditions could be obtained with the same Monte Carlo program. For example, the relaxation of the asymmetric bi-modal distribution functions used by Mott-Smith to describe shock wave structure could be studied.

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## 1. Introduction

The series of internal CSL reports, "Numerical Studies of Strong Shock Waves",[1-6] describes successive steps in our efforts to calculate the velocity distribution functions within a shock wave by solving the Boltzmann equation. We have shown that Nordsieck's Monte Carlo method of evaluating the collision integral in the Boltzmann equation appears to be both reliable and feasible. Earlier methods of evaluation have been less accurate and efficient.[7,8,9] The chief difficulty yet remaining to be overcome in the shock problem is that of insuring an adequate rate of convergence of the iterative method of solution of the Boltzmann equation. We therefore decided to apply the Monte Carlo method to a simpler problem than the shock wave in order to

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1. Numerical Studies of Strong Shock Waves. Part I. Illiac Solutions of a Boltzmann Difference Equation by Nordsieck's Method. B. L. Hicks and J. K. Aggarwal. CSL Report I-111. (1962)

2. _____. Part II. Results of Illiac Calculations. B. L. Hicks and J. K. Aggarwal. CSL Report I-117. (1963)

3. _____. Part III. Studies of the Monte Carlo and Integration Programs. B. L. Hicks. CSL Report I-122. (1963)

4. _____. Part IV. Description of the 1604 Program. J. K. Aggarwal and B. L. Hicks. CSL Report I-123. (1963)

5. _____. Part V. Equations and Scaling. B. L. Hicks. CSL Report I-124. (1963)

6. _____. Part VI. Subroutines and Tables. B. L. Hicks and M. A. Smith. CSL Report I-125. (1964)

7. "Molecular Dynamics by Electronic Computers". B. J. Alder and T. Wainwright in Transport Processes in Statistical Mechanics (Interscience Publishers, 1958), pp. 97-131.

8. "Investigation of the Many Body-Problem by Electronic Computers", B. J. Alder and T. Wainwright, in The Many Body-Problem (Interscience Publishers, 1963), pp. 511-522.

9. G. A. Bird, "Approach to Translational Equilibrium in a Rigid Sphere Gas". Phys. of Fl. 6, 1518 (1963).

demonstrate at once the utility of the method in a real problem and to learn from this exercise some new tricks to use on the shock structure problem.

We chose at Nordsieck's suggestion the simpler problem of calculating the translational relaxation of a uniform gas. In particular, we chose as the initial out-of-equilibrium condition a bimodal velocity distribution. This condition resembles that which obtains within a shock wave, and could be made more like a shock wave by simple extensions of the calculations reported here. Hence we call our problem of relaxation the "pseudo-shock" problem.

We have solved the Boltzmann equation numerically for initial conditions ranging from near thermal equilibrium to very far from thermal equilibrium. The numerical results are readily interpretable physically and suggest a new numerical technique that should be useful in the shock wave problem.

We are indebted to Mrs. Margaret Smith who has performed most of the programming and data reduction for our study of the pseudo-shock.

## 2. Formulation of the problem

We shall treat the behavior of a uniform monatomic gas that is not in thermal equilibrium. We shall consider hard sphere molecules of diameter $\sigma$ and mass m. Molecules with other force fields can be studied if their differential cross sections are known. We shall suppose that there are no external forces. The behavior to be considered is then that of a simple translational relaxation which is governed by the Boltzmann equation.

One set of units will be used in the body of the paper. A second set, "machine units", will be used in the Sect. 4.3. (See also Part I(1).) In the first set, the units are the values, denoted by the subscript 1, of various properties of a reference gas. Thus $n_1$, $T_1$ are the units of number density and temperature. The unit of length $\ell_1 = 1/(2\pi n_1 \sigma^2) =$ $((\text{mean free path})_1/\sqrt{2})$. The unit of velocity

$c_1 = (2\pi kT_1/m)^{\frac{1}{2}} = (\text{mean speed})_1 \times (\pi/2)$. The unit of time is therefore $(\text{mean free time})_1 \times (\sqrt{2}/\pi)$ and of the velocity distribution function is $n_1/c_1^3$. In these units the Boltzmann equation may be written

$$df/d\tau = a - bf = \int (FF' - ff')|\vec{N}\cdot\vec{v}_r|\, d\vec{v}'\,(d\vec{N}/4\pi) \qquad (2\text{-}1)$$

where $f = f(\vec{v},\tau)$ is the time-dependent velocity distribution function, $\tau$ is the time variable, $\vec{N}$ gives the direction of the line of centers during a collision, $\vec{v}_r = \vec{v}' - \vec{v}$, and $f$, $f'$, $F$, $F'$ denote the four values of $f$ corresponding to the four velocities $\vec{v}$, $\vec{v}'$, $\vec{V}$, $\vec{V}'$ characterizing a binary collision.

We specify, as the initial condition at $\tau = 0$, a symmetrical bimodal velocity distribution function for a spatially uniform gas

$$f(\vec{v},0) = f_0 = \frac{1}{2}\left\{\exp\left[-\pi(\vec{v}-\vec{i}u)^2\right] + \exp\left[-\pi(\vec{v}+\vec{i}u)^2\right]\right\} . \qquad (2\text{-}2)$$

At all later times the velocity distribution function depends only upon $\tau$ and the velocity components $(v_x, v_\perp)$ which are cylindrical polar coordinates in velocity space. In our units the parameter $u$ is related to a Mach number by the equation

$$M = (6\pi/5)^{\frac{1}{2}} u \quad . \qquad (2\text{-}3)$$

For $M \ll 1$ the gas described by $f_0$ is almost in thermal equilibrium at temperature $t = 1$ and with number density $n = 1$. For $M \gg 1$, the gas described by $f_0$ is very far from equilibrium, and, in fact, consists of two oppositely directed streams of gas, each at temperature $t = 1$ moving essentially parallel to the $x$ axis at a speed large compared to the thermal velocity.

We shall be interested in the behavior of the velocity distribution function $f$, the collision integral $(a\text{-}bf)$, the "lateral" temperature

$$T_\perp/T_1 = t_\perp = (\pi/n)\int v_\perp^2 f d\vec{v} \tag{2-4}$$

and the Boltzmann function

$$H = \int f \log f \, d\vec{v} \quad . \tag{2-5}$$

The number density $n \equiv 1$ throughout the relaxation process. The reduced temperature

$$T/T_1 = t = (2\pi/3n)\int v^2 f \, d\vec{v} = 1 + (5/9)M^2 = 1 + \frac{2}{3}\pi u^2 \tag{2-6}$$

is likewise constant throughout the relaxation process.*

The initial and final ($\tau \rightarrow \infty$) values of $t_\perp$ are equal, respectively, to 1 and t. The initial values of H can be computed analytically for two values of M:

$$H(0) = -\frac{3}{2}, \qquad M = 0 \tag{2-7}$$

$$H(0) = -\frac{3}{2} - \ln 2 \ , \quad M = \infty \ . \tag{2-8}$$

For other values of M, H(0) must be computed by numerical quadrature. The asymptotic value of H is given by

$$H(\infty) = -\frac{3}{2}(1 + \ln t) \tag{2-9}$$

corresponding to the asymptotic velocity distribution function

$$f_\infty(\vec{v}) = f_\infty = t^{-\frac{3}{2}} \exp(-\pi v^2/t) \ . \tag{2-10}$$

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*As we shall see later (and compensate for) n and t do not remain exactly constant during the <u>numerically</u> <u>calculated</u> relaxation process.

## 3. Theoretical Expectations

From Boltzmann's Theorem we know that

$$dH/d\tau < 0 \tag{3-1}$$

during the relaxation. The asymptotic value of H for an equilibrium gas with given t and for n = 1 is given by Eq. (2-9), and according to Eq. (3-1) this value must be the lowest value reached by H during the relaxation.

Let $\delta f = \delta f(\vec{v},\tau)$ represent the departure of the velocity distribution function from $f_\infty = f(\vec{v},\infty)$, its equilibrium value. Then

$$f = f_\infty + \delta f \tag{3-2}$$

and

$$t_\perp = t + (\pi/n)\int v_\perp^2\, \delta f\, d\vec{v} \quad . \tag{3-3}$$

An equation similar to (3-3) holds for any moment of f.

It will be convenient to interpret the time scale and collision rates in terms of the behavior of the equilibrium gas, described by $f_\infty$. We may expect the time constant for the equilibrium gas and for the asymptotic part of the relaxation to be inversely proportional to the mean molecular speed and therefore to $t^{-\frac{1}{2}}$ . The asymptotic relaxation for different Mach numbers should then be similar when plotted against $(t^{\frac{1}{2}}\,\tau)$. The number of collisions $\mathcal{N}$ suffered by a molecule in the equilibrium reference gas in (reduced) time $\Delta\tau$ is

$$\mathcal{N} = (\sqrt{2}/\pi)t^{\frac{1}{2}}\ \Delta\tau = 0.450\, t^{\frac{1}{2}}\ \Delta\tau \ . \tag{3-4}$$

The relaxation will be almost complete when $(t^{\frac{1}{2}}\tau) >> 10$. In this asymptotic range, $|\delta f/f_\infty| << 1$ and

$$H \cong H_\infty + \frac{1}{2}\int \delta f^2 f_\infty^{-1} (1 - \delta f/3f_\infty)\, d\vec{v} + \ldots \quad . \tag{3-5}$$

The term in $(\delta f)$ is missing from Eq. (3-5) because n and t are constant during the relaxation. Offerhaus[10] has discussed the $(\delta f)^2$ term but not the $(\delta f)^3$ term in this equation.

To get a more detailed view of the relaxation process let us describe the process approximately by the Krook model,[11] in which the Boltzmann equation is replaced by

$$df/d\tau = b(\mathcal{F} - f) . \tag{3-6}$$

In this equation $\mathcal{F}$ is a Maxwell-Boltzmann distribution function having the same (constant) values of n and t as does the (non-equilibrium) function f. Therefore, $\mathcal{F} = f_\infty$ is independent of $\tau$. The solution of Eq. (3-6) then is

$$f = f_\infty + (f_o - f_\infty)e^{-b\tau} \tag{3-7}$$

where b may or may not depend upon $\vec{v}$, according to the nature of the Krook model. Notice that f, in Eq. (3-7), is a linear combination of $f_o$ and $f_\infty$. We may thus say that Eq. (3-7) corresponds, for our translational relaxation problem, to a Mott-Smith model of the process as well as to a Krook model.

We now have an explicit form for $\delta f$ to use,

$$\delta f = (f_o - f_{oo})e^{-b\tau} \quad , \quad (t^{\frac{1}{2}}\tau \gg 1) . \tag{3-8}$$

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10. M. F. Offerhaus, Theory of Relaxation Phenomena in a Monatomic Gas. Akad. 64, 115 (1961), see Sect. 5.

11. Bhatnaghar, Gross, and Krook. "A Model for Collision Processes in Gases." Phys. Rev. 94, 511 (1954).

The relaxation of $t_\perp$ (or other moments) is similar to that of f:

$$t_\perp = t + (\pi/n)\int (f_o - f_\infty) v_\perp^2 e^{-b\tau} d\vec{v} . \tag{3-9}$$

But for large enough times, namely, for

$$\left| \delta f/3f_\infty \right| = (f_o - f_\infty) e^{-b\tau}/3f_\infty \ll 1 , \tag{3-10}$$

we find that

$$H = H_\infty + \frac{1}{2}\int e^{-2b\tau}(f_o - f_\infty)^2 f_\infty^{-1} d\vec{v} . \tag{3-11}$$

The time constant $b(\vec{v})$ of the (asymptotic) relaxation for each velocity bin increases with increase of the speed v. Let $b_1$ be the smallest value of b. Then for large enough times the relaxation of the corresponding velocity bin will dominate the relaxation process and we may write in place of Eqs. (3-9), (3-11)

$$t_\perp = t + (1-t)e^{-b_1\tau} \tag{3-12}$$

$$H = H_\infty + \frac{1}{2} e^{-2b_1\tau} \int (f_o - f_\infty)^2 f_\infty^{-1} d\vec{v} . \tag{3-13}$$

Results of the same form follow from the alternative assumption that b = constant. For example, we may assume that $b_1$ in the Krook model corresponds to the value b(0) for the equilibrium gas; then

$$b_1 = b(0) = t^{\frac{1}{2}}/\pi . \tag{3-14}$$

Insofar as the Krook model is valid for the asymptotic part of the relaxation process we thus can predict that <u>the time constant $b_H$ for the relaxation of H is one-half as large as the time constant $b_\perp = b_1$ for the asymptotic relaxation of $t_\perp$</u>. It may also be shown for the Krook model that the term

in $\delta f^3$ is negative, for large enough values of M, which has the apparent effect of making $b_H/b_\perp > 1/2$ when $b_H\tau \sim 1$. Even without appealing to the Krook model we can show that this is a reasonable result when we look at the $(\delta f)^3/f_\infty^2$ term in the integrand of Eq. (3-4). This term behaves near a residual peak like $t^3$ and elsewhere like $t^{-\frac{3}{2}}$. Remembering that $\int \delta f d\vec{v} = 0$, we see that for large enough t, the integral of $\delta f^3/f_\infty^2$ is positive and the corresponding contribution to H is negative.

For large values of M we can also make a prediction about the <u>early</u> part of the relaxation process. In this case few collisions occur except between molecules moving with velocities u and (-u) nearly parallel to the x axis. For $t^{\frac{1}{2}}\tau \ll 1$ only a small number of molecules will have collided and these will be distributed uniformly in velocity space along the circle v = u. We may expect then (for $M \gg 1$ and $(t^{\frac{1}{2}}\tau) \gg 1$) that we will see in isoline plots of f a "bridging" along a circular arc between the two delta functions at $v_x = \pm u$, $v_\perp = 0$.

It should be noted that one analytical treatment[12] of translational relaxation has been based upon superposition throughout the relaxation of two Maxwell-Boltzmann distributions the separation of whose centers continuously decreases. This model cannot account for the directional randomization just discussed, but addition of a third Maxwell-Boltzmann distribution might yield asymptotic results similar to those suggested by the Krook model.

We are now ready to consider the numerical methods used in solving the translational relaxation problem.

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12. K. Suchy, "New Methods in the Kinetic Theory of Rarified Gases." Ergeb. exakt. Naturwiss. 35, 103 (1964).

## 4. Numerical Methods

### 4.1 Evaluation of the Collision Integral by Monte Carlo Sampling

The most difficult part of the translational relaxation problem is evaluation of the collision integral. It is fortunate, since no other suitable method (analytical or numerical) is yet available, that Nordsieck's Monte Carlo method is well developed.

The method was described in the first report of the series.[1] The collision integral is first replaced by an integral over a finite region of velocity space that is of volume R and that includes most of the molecules. The average value of the integrand over this region is then approximated by the average of a large and fair sample of N values of the integrand. The value of the collision integral is then given by the product of this average value with the volume R. The integrand is a function of eight independent variables derived from $\vec{v}$, $\vec{v}'$, and $\vec{n}$. Nordsieck's Monte Carlo method insures fairness of the sampling in the eight-dimensional space of these variables. The sampling and Monte Carlo quadrature make use of 226 velocity bins in the $(v_x, v_\perp)$ plane.

In a numerical solution of the Boltzmann equation, it is the speed and accuracy of the evaluation of the collision integral that must be our primary concern before we look at other characteristics of the over-all method of solution. For samples of moderate size and velocity distributions that cover about 200 velocity cells, statistical fluctuations contribute the only significant error, for the statistical error is then much larger than the quadrature error. (Truncation error is generally small except for large values of the speed v where the collision integral itself is small.) Thus, with our present Monte Carlo program,* the calculation of 226 values of (a-bf), for a

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*Detailed tests of this program have not yet been described in reports. Tests of earlier programs are described in Part III.[3]

sample of $N = 10^4$ collisions, is performed in 50 sec. on the CDC 1604 computer and yields statistical errors (expressed as probable errors) in a and bf individually of $\pm 15\%$. The bias, owing to quadrature error, amounts to $\pm 2\%$ in uncorrected a or bf for a well-covered velocity space for an equilibrium gas. The bias in (a-bf) is not now directly determinable for a non-equilibrium gas but is reduced by the method described in Sec. 4.4. We would like to emphasize that some bias in (a-bf), caused by quadrature error, is to be expected whether the numerical integration uses sampling techniques or not.

The computing time is proportional to N, and the statistical error is proportional to $N^{-\frac{1}{2}}$. For many calculations it is not practical nor is it necessary to reduce the statistical error to the same level as the bias. We have obtained significant results in the relaxation problem with relatively small samples ($N = 10^4$).

For $M \gg 1$, only a few velocity bins, in effect, are used in Monte Carlo (or other) numerical evaluation of the collision integral. The large resulting quadrature error then presents the primary difficulty in solving the relaxation problem adequately for large Mach numbers. (See Sect. 6.32.)

## 4.2 Integration of the Boltzmann Equation

Consideration of the various sources of error and of factors influencing the computing speed indicated that Euler quadrature in the time variable would give appropriate accuracy and speed. For each velocity bin the integration formula is

$$f(\tau_1+\Delta\tau) = f(\tau_1) + \Delta\tau(df/d\tau)\Big|_{\tau_1} . \qquad (4\text{-}1)$$

In view of the discussion in Section 3 we chose $\Delta\tau$ to be approximately proportional to $t^{-\frac{1}{2}}$ so that quadrature errors in the forward integration are approximately equal, on a fractional basis, for different Mach numbers.

We may add two further notes about the forward integration process. A process of higher order than the Euler would require recalculation of (a-bf) one or more times before a step in time is made. Improvements in accuracy of the time-wise integration must take into account, however, that by far the most time-consuming part of the whole problem, even with the help of a Monte Carlo process, is the evaluation of the collision integral. Thus, (see Sect. 4.1) one forward step in time takes 50 sec., for a sample of $10^4$ collisions. We can, however, on the basis of a reasonable assumption, easily correct the results of the Euler integration and thereby achieve about the same accuracy in calculation of $t_\perp$ and H as though we had used a higher order integration process.

The assumption used is that <u>each</u> function (f, $t_\perp$ and H) which we later discuss is nearly an exponential function, $\exp(-\beta t^{\frac{1}{2}}\tau)$. For the function $f(\tau)$, for example, we may then write the expression for the derivative at the mid-point of an interval as

$$f'(\tau + \tfrac{1}{2}\Delta\tau) = -\beta t^{\frac{1}{2}} f(\tau + \tfrac{1}{2}\Delta\tau) \cong -\beta t^{\frac{1}{2}} f(\tau)\,[1 - \tfrac{1}{2}\beta t^{\frac{1}{2}}\Delta\tau] \quad . \tag{4-2}$$

Each increment $\Delta f$ from an Euler integration should then be multiplied by the (constant) correction factor $[1 - \frac{1}{2}\beta t^{\frac{1}{2}}\Delta\tau]$ and logarithmic slopes should be corrected by the same factor. We assume that the logarithmic slopes of the functions $t_\perp$ and H should be corrected by the factors $[1 - \frac{1}{2}\beta_\perp t^{\frac{1}{2}}\Delta\tau]$ and $[1 - \frac{1}{2}\beta_H t^{\frac{1}{2}}\Delta\tau]$ where $\beta_\perp$ and $\beta_H$ are determined later. The correction made of the slopes of the H curves is greater than that of the $t_\perp$ curves but is less than 15%. Higher order corrections would not change the values of the slopes by more than 1%.

## 4.3 Integrals involving f and (a-bf)

As in our earlier work[1,5] we calculate n, nt, $nt_\perp$ and H (each of which involves integration of f over velocity space), and $dn/d\tau$, $d(nt)/d\tau$ (each of which involves integration of (a-bf) over velocity space) by numerical quadratures in velocity space. Combined quadrature and truncation errors have been reduced to less than 1% for all values of M for large values of $(t^{\frac{1}{2}}\tau)$, but, for large Mach numbers, $(M \geq 4)$, it is not possible, for a given number of velocity bins (226 in our case), to keep the quadrature errors this small for $(t^{\frac{1}{2}}\tau) < 1$. (See discussion of Table II in Sect. 6.2.)

To facilitate control of the truncation error we introduced two related parameters $K_1$ and p. The parameter $K_1$ is used to scale the variable $\vec{v}$ so as to "fill" the velocity space, for a given function f. Thus

$$\vec{v}_m = K_1 \vec{v} \tag{4-3}$$

where 226 fixed values of $(v_x, v_\perp)_m$ (velocity components in "machine" units) describe the velocity cells in the truncated region R over which numerical integrations are carried out. Though it is not in principle necessary, we keep $K_1$ fixed during the time-wise integration of the Boltzmann equation for any one value of M.

As a simple measure of truncation error (in calculating integrals over f) we use the integer p in the equation

$$f_\infty(24/K_1) = 10^{-p}, \tag{4-4}$$

$v_m = 24$ being the radius of the spherical region R. Combination of Eqs. (4-4) and (2-10) then gives a value of $K_1$ for each value of M or t. We took p to be 4.

We have not examined the fractional truncation error in the evaluation of (a-bf). We would expect it to be less than the corresponding errors in integrals over f because the integrand of the collision integral contains products of velocity distribution functions and therefore decreases much more rapidly than f as the speed v increases.

## 4.4 Least Square Adjustment of Calculated Collision Integrals

As we have noted above, some bias in values of the collision integral calculated by numerical quadrature is unavoidable. To reduce the resultant accumulation of errors in the forward integration of the Boltzmann equation in time we have devised a least square adjustment of the collision integrals that are calculated by Monte Carlo sampling. This method is preferable to the "moment correction" method[1,4,5] used for the shock problem two years ago because it less often produces negative and therefore unacceptable values of f.

Let us first consider the values of n and t calculated from the f's generated by our numerical treatment of the Boltzmann equation. These values of n and t would remain constant throughout the relaxation process if there were no error in calculating them. We will go far toward enforcing constancy of these values if we adjust the values of (a-bf) as little as possible, in a least square sense, while imposing the two conditions

$$dn/d\tau = \int (df/d\tau)d\vec{v} = 0 \qquad (4\text{-}5)$$

$$d(nt)/d\tau = (2\pi/3)\int v^2(df/d\tau)d\vec{v} = 0 \qquad (4\text{-}6)$$

Both the Monte Carlo calculation of the function $(df/d\tau)$ and the numerical quadrature used to approximate the integrals in Eq. (4-5,6) introduce errors in the values of $dn/d\tau$ and $d(nt)/d\tau$. As noted before, the adjustment process therefore maintains the constancy of the computed values of n and of t.

The least square condition, subject to Eqs. (4-5) and (4-6), is

$$\delta \sum_{s=0}^{225} (p_s - P_s)^2 p_s^{-2} = 0 \qquad (4\text{-}7)$$

in which $p_s$ and $P_s$ are the values of $df/d\tau$ (for the sth velocity bin) before and after adjustment. Solution of the least square problem yields a simple explicit formula for $P_s$ in terms of moments of $df/d\tau$ that are approximated by weighted sums. Note that we minimize the mean square value of the <u>fractional</u> adjustment of $p_s$, a procedure that is consistent with a characteristic of Nordsieck's Monte Carlo method, namely, the approximately constant fractional error of the values of $df/d\tau$ that it produces.

We checked the effectiveness of the correction method by obtaining Monte Carlo solutions of the Boltzmann equation for M = 0 both with and without the correction of (a-bf). For M = 0 the gas is <u>initially</u> in equilibrium so that properties of the gas that are calculated by the Monte Carlo method should deviate from the equilibrium values of these properties only because of fluctuations and bias in the Monte Carlo method.

With a program which uses the correction method, the f and a isolines for M = 0 differ in only a few bins from the equilibrium isolines. This is true both after two and 20 steps in time. The isolines of (a-bf) indicate probable errors of about 24% relative to a. When no corrections of (a-bf) have been made then t, $t_\perp$ and $|H|$ increase by 1.6, 1.6 and 1.7%, respectively, after the 20 steps in time. Correction of (a-bf) yields of course a constant computed value of t (low by 0.3% owing to quadrature and truncation error in integrating f to get t) and yields values of $t_\perp$ and H that fluctuate <u>near</u> the equilibrium values. These fluctuations in $t_\perp$ amount to ~0.4% and in H to ~0.05%.

The mean value of $|H|$ as calculated from the corrected (a-bf) is low by 0.3% (quadrature and truncation error over f) and perhaps shows a slight downward bias amounting to 0.1% in 20 steps in time. The size of the fluctuations will be used later in interpreting the pseudo-shock calculations.

These results show that the least square adjustment of the values of (a-bf) does indeed reduce the trends away from equilibrium that are produced by unavoidable slight bias in the Monte Carlo (or other) calculation of (a-bf).

### 4.5 Monte Carlo Fluctuations

As in an earlier investigation[3] we wished to study statistical variation of quantities that had been calculated with the help of Monte Carlo sampling. Therefore we made four runs of the same type but each run with a different and independent sample. For each run we chose to use a sample of $N = 10^4$ collisions for each of ten steps in time, starting at $\tau = 0$ for each Mach number, and also at $\tau = 10\Delta\tau$, so that we could judge the effects of the Mach number and of the phase of the relaxation upon the variances among the runs.

We shall be concerned chiefly in later sections with the variance of the derivatives of $t_\perp$ and H as functions of $(t^{\frac{1}{2}}\tau)$.

## 5. Parameters

The parameters that define the numerical treatment of the translational relaxation process are $\Delta\tau$, N, p, and the first random number used in generating a sequence of independent samples for a given run. Except as specified otherwise, the sequences of samples were wholly independent of one another. There is only one physical parameter governing the relaxation process, namely M. Parameters used in the various runs are summarized in Table I.

Table I. Summary of Pseudo Shock Calculations

| M | interval $\Delta\tau$ | $t^{\frac{1}{2}}\,\Delta\tau$ | Range of $(\tau/\Delta\tau)$ | p | no. of runs (a) | N |
|---|---|---|---|---|---|---|
| 0 | .25 | .25 | 1-20 | 4 | 1 | 10,923 |
| | | | 1-20 | | 1 (b) | |
| .5 | .25 | .2668 | 1-10 | 4 | 4 | 10,923 |
| | | | 11-16 | | 1 | |
| | | | 11-30 | | 1 | |
| 1 | .25 | .3118 | 1-10 | 4 | 4 | 10,923 |
| | | | 11-20 | | 4 | |
| | | | 11-30 | | 1 | |
| 2 | .25 | .4488 | 1-10 | 4 | 4 | 10,923 |
| | | | 11-20 | | 4 | |
| | | | 11-30 | | 1 | |
| | .125 | .2244 | 1-10 | 4 | 1 | 43,691 |
| 4 | .125 | .3931 | 1-10 | 4 | 4 | 10,923 |
| | | | 11-20 | | 4 | |
| | | | 11-30 | | 1 | |
| | .0625 | .1965 | 1-4 | 4 | 1 | 43,691 |
| 6 | .0625 | .2864 | 1-20 | 4 | 1 (c) | 10,923 |
| | | | 1-20 | 3 | 1 (c) | |
| | | | 1-20 | 2 | 1 (c) | |
| | | | 1-10 | 4 | 3 | |
| | | | 11-20 | | 3 | |
| | | | 21-30 | | 1 | |
| 10 | .0625 | .4700 | 1-10 | 4 | 4 | 10,923 |
| | | | 11-20 | | 4 | |
| | | | 21-30 | | 1 | |

(a) All runs were made with independent samples unless indicated otherwise.

(b) No (a-bf) corrections.

(c) These three runs were made with the same sample.

## 6. Results and Discussion

### 6.1 Preliminary Comparison with Theoretical Expectations

In interpreting our computational results we shall be interested in the behavior of the lateral temperature $t_\perp$ and the Boltzmann function H, and, to a lesser extent, in the detailed appearance of isoline plots of f, a, and (a-bf). The behavior of $t_\perp$ and H is shown in Figs. 1 and 2 for five values of the Mach number M. In each figure, the abscissa is $t^{\frac{1}{2}}\tau$ where t is the (reduced) equilibrium temperature given by Eq. (2-6) and $\tau$ is the (reduced) time variable.* The ordinates in Figs. 1 and 2 represent the absolute value of the differences $(t_q(0)-t_{\perp M}(\tau))$ and $(H'(\infty) - H_M(\tau))$, calculated from the Monte Carlo results, where $t_q(0)$ and $H'(\infty)$ are the asymptotic values of $t_\perp$ and H. Discussion of the estimation of these and other asymptotic values will be deferred to later sections. Let us now state briefly what these figures show that was predicted in Sect. 3.

The numerical results do satisfy Boltzmann's Theorem, at least until the relaxing gas is close enough to equilibrium so that the Monte Carlo fluctuations produce fluctuations of H above and below the equilibrium value $H'(\infty)$. Except for M = 0.5, the range of $(H_M(\tau) - H'(\infty))$ before such deviations occur is two or more decades. Both $t_\perp$ and H (which are measures of departure from equilibrium) relax as though a single relaxation mechanism were effective <u>from the onset of the relaxation process</u>. Time constants for different values of M are proportional to $t^{-\frac{1}{2}}$, as indicated by the parallelism of the relaxation curves plotted with $t^{\frac{1}{2}}\tau$ on the abscissa. The time constant for relaxation

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*We recall that $0.450t^{\frac{1}{2}}\tau$ is the number of collisions that have occurred in reduced time $\tau$ in the reference gas. (See Eq. (3-4).)

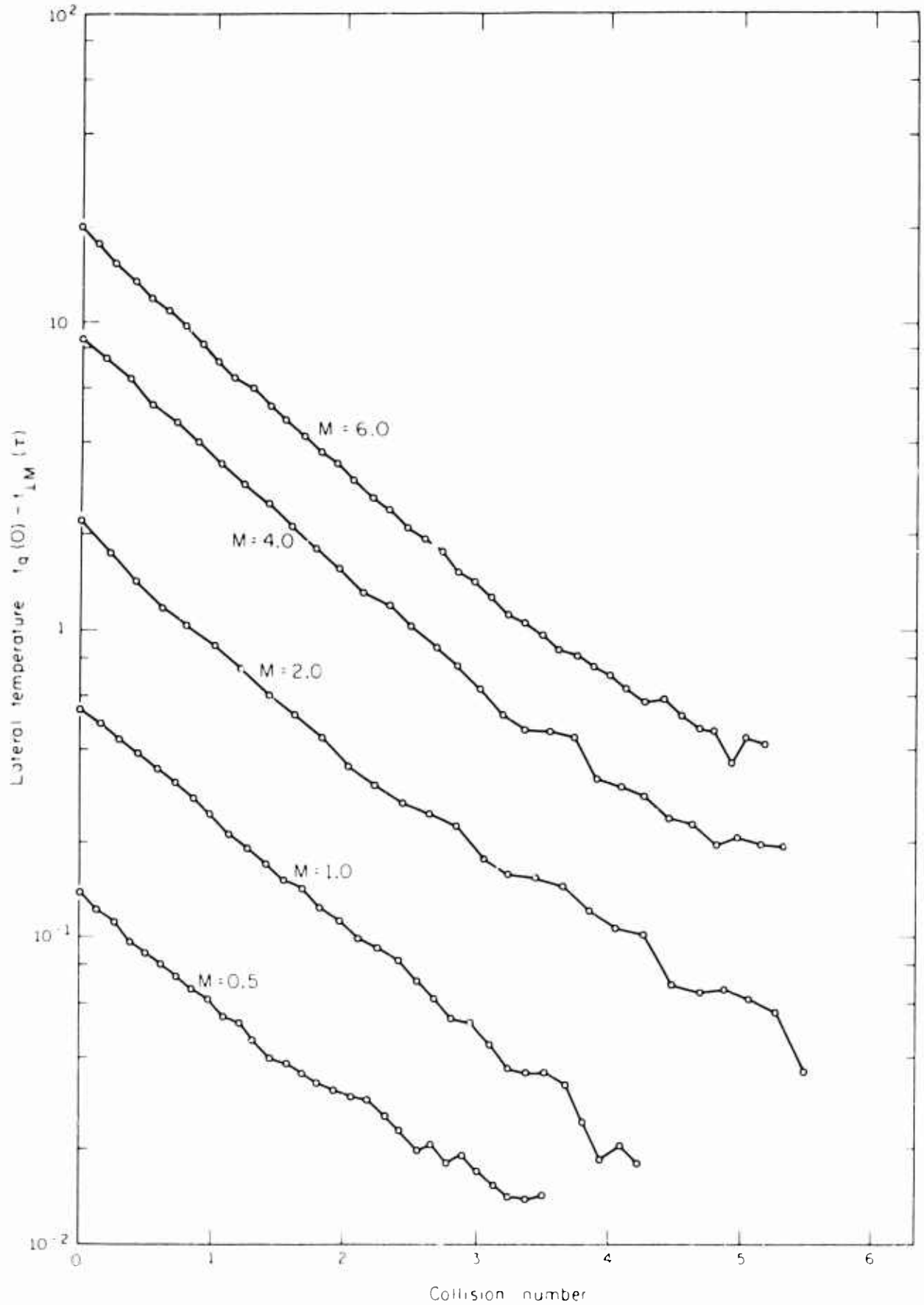


Figure 1. Translational relaxation of reduced temperature. The collision number is calculated for a reference gas which is in equilibrium and has the same total translational energy as the relaxing gas. Mach number M.

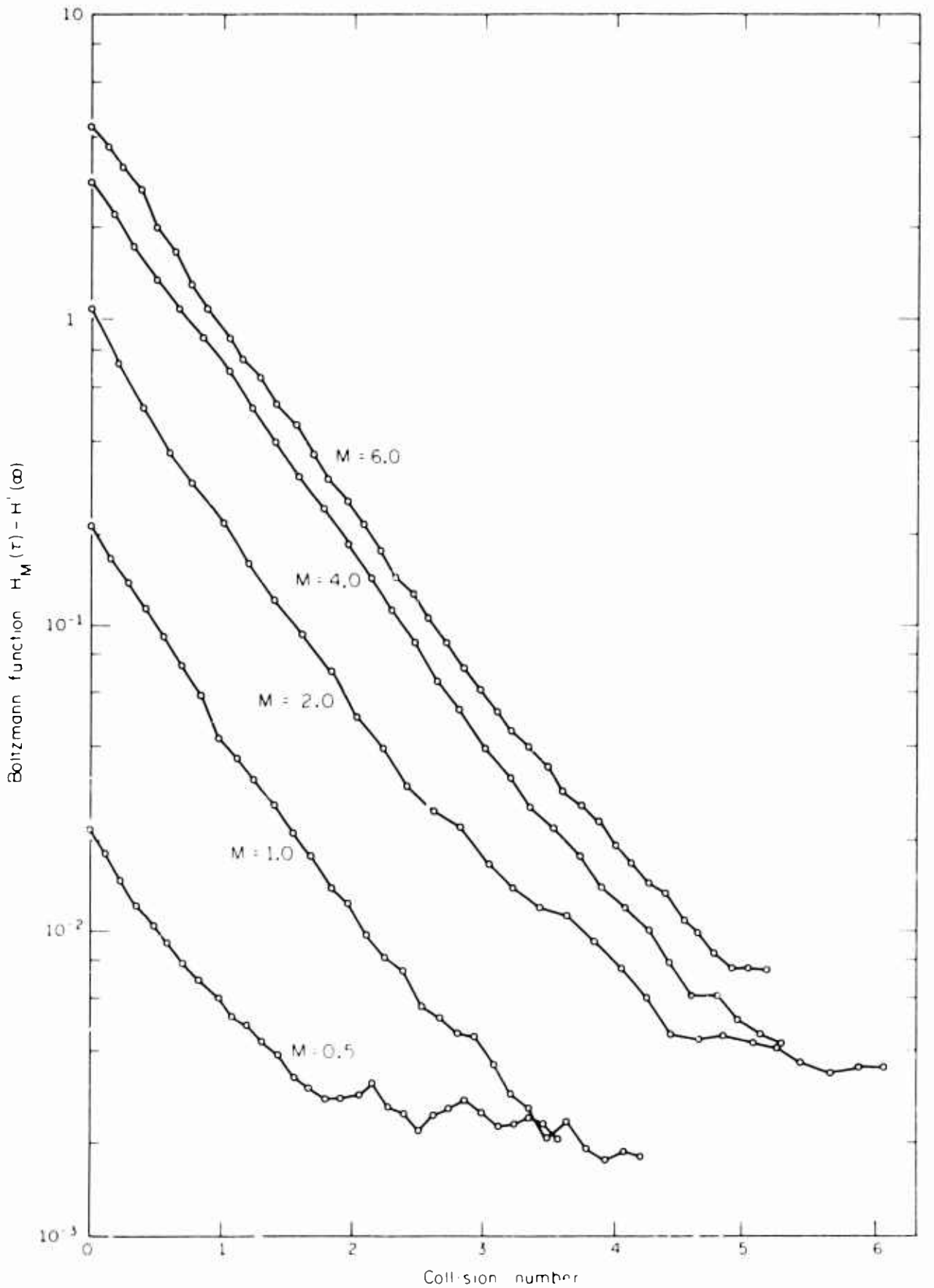


Figure 2. Translational relaxation of the Boltzmann function. The collision number is calculated for a reference gas which is in equilibrium and has the same total translational energy as the relaxing gas. Mach number M.

of H does appear to be about one-half as large as for the relaxation of $t_\perp$.

In Fig. 3 the predicted "bridging" is clearly visible in the f-isolines for M = 4. These isolines (see Table I) were calculated for $\Delta\tau = 0.0625$ corresponding to a collision of only one molecule in 11 in the reference gas, showing the sensitivity of Nordsieck's method. Our examination of the isolines for f, a and (a-bf) also shows that they approach, for $t^{\frac{1}{2}}\tau \gg 1$, the shapes characteristic of equilibrium, as we would expect.

Although a more careful discussion of these points will be given later, we can already see that agreement with the theoretical expectations gives considerable indirect support to the validity of our Monte Carlo solution of the Boltzmann equation for the pseudo-shock.

## 6.2 Asymptotic Behavior

Let us first examine the behavior of $t_\perp$ and H for large times, i.e. for $\tau \cong 20\ \Delta\tau$. We have made a number of different estimates, given in Table II, of both the initial and asymptotic values of $t_\perp$ and H. These estimates are derived from different combinations of analytical formulas, numerical integrations, and Monte Carlo calculations. It is necessary to consider various estimates of $n(\tau)$ and $t(\tau)$ as well as of $t_\perp(\tau)$ and $H(\tau)$.

Let us use the subscript a to indicate a wholly analytical calculation; the subscript q to indicate a result derived by numerical integration of an analytical $f(\vec{v},\tau)$ over $\vec{v}$; and the subscript M to indicate a result derived by numerical integration of a Monte Carlo $f(\vec{v},\tau)$ over $\vec{v}$. Initial and asymptotic values of the various estimates are indicated by the values 0 and $\infty$ of the argument $\tau$.

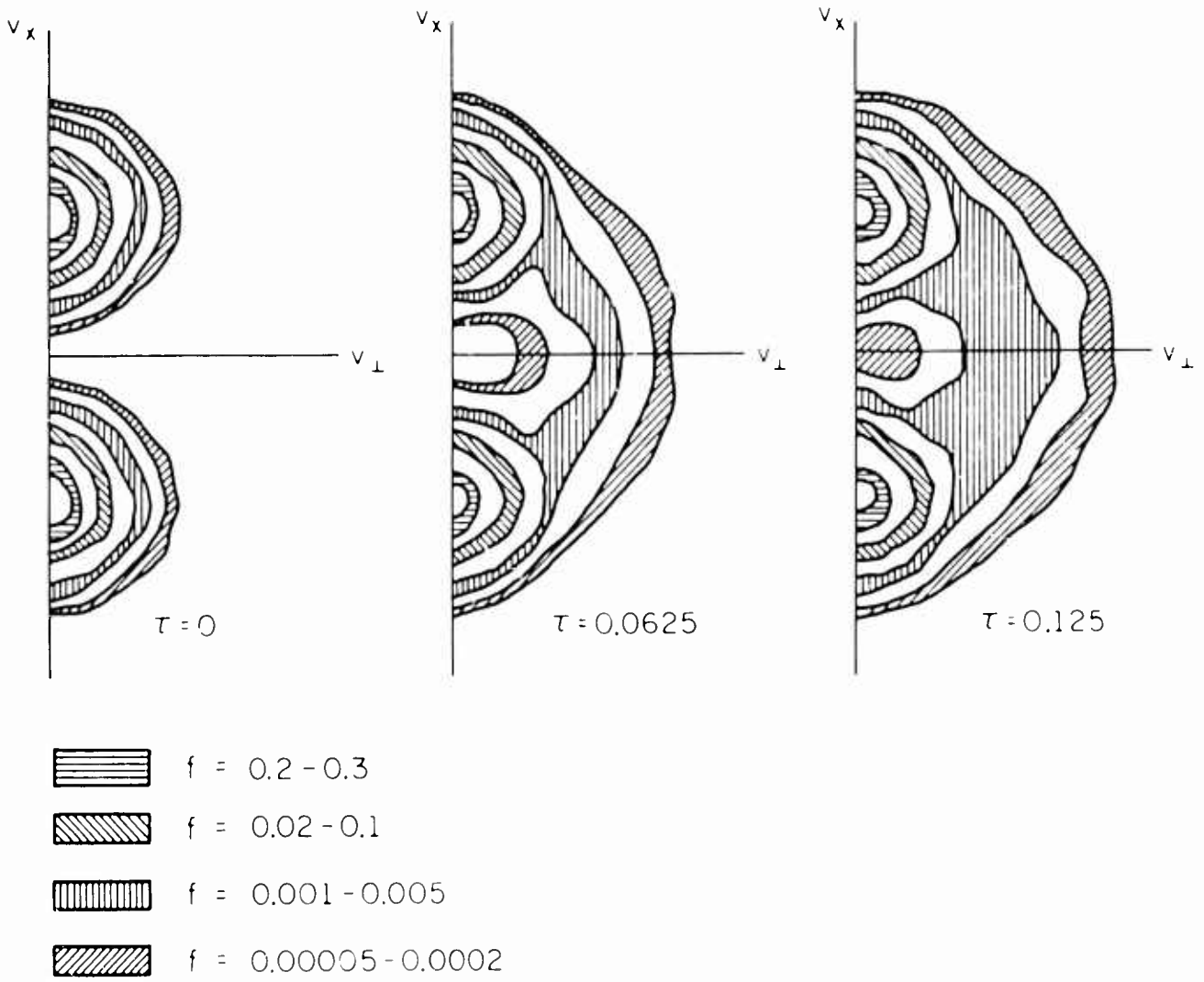


Figure 3. Early stages in the relaxation of the velocity distribution function f for a Mach number of 4.0. $v_x$ and $v_\perp$ are cylindrical polar coordinates in velocity space. The (reduced) time interval $\Delta\tau = 0.0625$ corresponds to a collision of one molecule in eleven in a reference gas.

Table II. Limiting Values of Macroscopic Properties of the Relaxing Gas

| 1. | 2. | 3. | 4. | 5. | 6. | 7. | 8. | 9. | 10. |
|---|---|---|---|---|---|---|---|---|---|
| $M$ | $n_a$ | $n_q(0)$ | $n_q(\infty)$ | $t_a$ | $t_q(0)$ | $t_q(\infty)$ | $t_{\perp q}(0)$ | $t_{\perp q}(\infty)$ | $t_{\perp M}(\infty)$ |
| 0.0 | 1.000 | .99973 | | 1.000 | .99743 | | .99736 | | |
| 0.5 | 1.000 | .99982 | .99956 | 1.1389 | 1.1363 | 1.1334 | .99817 | 1.1333 | 1.14 |
| 1.0 | 1.000 | 1.0002 | .99995 | 1.5556 | 1.5539 | 1.5500 | .99893 | 1.5499 | 1.55 |
| 2.0 | 1.000 | 1.0015 | 1.0012 | 3.2222 | 3.2201 | 3.2119 | .99691 | 3.2117 | 3.22 |
| 4.0 | 1.000 | 1.0148 | 1.0146 | 9.8889 | 9.8686 | 9.8436 | .96952 | 9.8429 | 9.87 |
| 6.0 | 1.000 | 1.0780 | 1.0777 | 21.000 | 20.865 | 20.813 | .83621 | 20.812 | 20.8 |
| 10.0 | 1.000 | 1.2914 | 1.2913 | 56.556 | 53.976 | 53.876 | .92132 | 53.871 | |
| $\infty$ | 1.000 | | | $\infty$ | | | | | |

| 1. | 11. | 12. | 13. | 14. | 15. | 16. |
|---|---|---|---|---|---|---|
| $M$ | $H_a(0)$ | $H_q(0)$ | $H_a(\infty)$ | $H_q(\infty)$ | $H'(\infty)$ | $H_M(\infty)$ |
| 0.0 | -1.5000 | -1.4958 | -1.5000 | | -1.4961 | |
| 0.5 | | -1.6696 | -1.6951 | -1.6873 | -1.6915 | -1.689 |
| 1.0 | | -1.9557 | -2.1628 | -2.1570 | -2.1614 | -2.160 |
| 2.0 | | -2.1797 | -3.2551 | -3.2528 | -3.2575 | -3.254 |
| 4.0 | | -2.1947 | -4.9371 | -4.9871 | -4.9923 | -4.989 |
| 6.0 | | -2.1861 | -6.0668 | -6.4430 | -6.4486 | -6.442 |
| 10.0 | | -2.8784 | -7.5528 | -9.3284 | -9.3331 | |
| $\infty$ | -2.1932 | | $-\infty$ | | | |

In the second column of Table II appear the analytical values of $n(\tau)$, namely $n_a$, which has the value unity at all times because the number of molecules is conserved. In column 3 is the estimate $n_q(0)$, obtained by numerical integration over the analytical values of $f(\vec{v},0)$ given by Eq. (2-2). Truncation errors are negative for $n_q(0)$ (as they are also for numerical integrations yielding estimates of $|H(\tau)|$ and of all the positive functions in Table II) and decrease as M increases. The quadrature errors in $n_q(0)$ are apparently positive and increase (unavoidably, for a fixed number of velocity bins) as M increases. The error in $t_q(0)$ (column 6) is negative and smaller in absolute value than the error in $n_q(0)$. (Note that numerical quadrature yields values of $(nt)$ and $(nt_\perp)$ rather than $t$ and $t_\perp$ directly.)

We must emphasize at this point that our digital computer solution of the Boltzmann equation produces and uses values of $t_\perp$, H, $dn/d\tau$ etc. that have been obtained by numerical integration. In "clamping" the values of $n(\tau)$ and $t(\tau)$, by the method described in Section 4.4, we are then fixing the values of $n_M(\tau)$, $t_M(\tau)$ at their <u>initial</u> values, $n_q(0)$, $t_q(0)$. As the translational relaxation proceeds, the quadrature errors (over $\vec{v}$) in H and $t_\perp$ decrease and are much less than 1% for all Mach numbers for $(t^{\frac{1}{2}}\tau) \gg 1$. (The quadrature errors in (a-bf) presumably decrease even more rapidly.) The proper interpretation of our relaxation calculations is then that we are following the <u>relaxation of a gas whose asymptotic density and temperature are $n_q(0)$ and $t_q(0)$</u>. We shall therefore base several estimates of the asymptotic values of other functions upon these values $n_q(0)$ and $t_q(0)$.

The velocity distribution function for a gas in thermal equilibrium and having the density and temperature $n_q(0)$, $t_q(0)$ is

$$f_\infty(\vec{v}) = n_q(0)[t_q(0)]^{-\frac{3}{2}} \exp[-\pi v^2/t_q(0)] \ . \qquad (6\text{-}1)$$

(Compare eq. (2-10).) Numerical integration over this function gives the values $n_q(\infty)$, $t_q(\infty)$ listed in columns 4 and 7 of Table II. The differences between $n_q(0)$ and $n_q(\infty)$ and between $t_q(0)$ and $t_q(\infty)$ are very small, which testifies to the small combined truncation and quadrature errors of our numerical integration over $\vec{v}$ for functions $f(\vec{v})$ that "fill" properly the part of $\vec{v}$ space we use for numerical integration.

Having given this much detailed discussion of the quantities appearing in the first seven columns of Table II, we can discuss rather briefly the related quantities listed in columns 8, 9, 11, 12, 13, 14, 15 of the Table. The initial values of $t_{\perp q}(0)$ in column 8 exhibit small deviations from the correct value $t_{\perp a} \equiv 1$ for low Mach numbers and larger errors for high Mach numbers much as did $t_q(0)$. Also, as we might expect, $t_{\perp q}(\infty)$ in column 9 agrees very well with $t_q(\infty)$ for all values of M.

There seems to be no analytical formula for $H_a(0)$ as a function of M. The initial and asymptotic ($M \rightarrow \infty$) values shown in the Table in column 11 are, however, given by the Eqs. (2-7,8). Note the small range of H as compared to that of t. The initial values $H_q(0)$ obtained by numerical integration over $\vec{v}$ are given in column 12 and show large departures from the correct values only for M = 10. Exact values of $H_a(\infty)$ (column 13) are given by Eq. (2-9) and may be compared with the values of $H_q(\infty)$ (column 14) obtained by numerical integration of $[f(\vec{v},\infty)\ln f(\vec{v},\infty)]$ over $\vec{v}$. The agreement is good except, as for M = 6, 10, where $n_q(0)$ is much different from unity. In view of our earlier discussion a more useful comparison is that between $H_q(\infty)$ and

$$H'(\infty) = n_q(0)[\ln n_q(0) - 1.5 \ln t_q(0) - 1.5] \qquad (6\text{-}2)$$

As we would expect, these two sets of values of $H(\infty)$ agree within much less than 1%.

We are now ready to discuss the behavior of the relaxing gas as determined from the Monte Carlo calculations. From our discussion in Section 3 we expect that $t_{\perp}(\tau)$ and $H(\tau)$ will each, to a first approximation, relax exponentially to their equilibrium values. To explore this possibility we plotted $[t_q(0) - t_{\perp M}(\tau)]$ and $[H_M(\tau) - H'(\infty)]$ on logarithmic scales vs. $(t^{\frac{1}{2}}\tau)$ on a linear scale as in Figures 1 and 2. For analysis of the early part of the relaxation process the asymptotic values chosen for subtraction from $t_{\perp M}(\tau)$ and $H_M(\tau)$ need be values only approximately equal to $t_q(0)$ and $H'(\infty)$. For the later parts of the relaxation, where the departure from the equilibrium values is small, it is necessary to choose these values to be $t_q(0)$ and $H'(\infty)$ (or other values such as $t_{\perp q}(\infty)$ and $H_q(\infty)$ that approximate closely to them).

The straight and parallel parts of the curves in Figures 1 and 2 will be discussed in a later section; we are concerned here only with the apparent asymptotic behavior* of the functions $t_{\perp M}(\tau)$ and $H_M(\tau)$. From these curves we derived estimates of the asymptotic values of $[t_q(0) - t_{\perp M}(\infty)]$ and of $[H_M(\infty) - H'(\infty)]$ and from these calculated values of $t_{\perp M}(\infty)$ and $H_M(\infty)$ as given in columns 10 and 16 of Table II. The values of $t_{\perp M}(\infty)$ are equal, within the uncertainty of estimating them (say 0.3%), to the values of $t_q(0)$. The values of $H_M(\infty)$ for $M \leq 10$, are equal to the values of $H_q(\infty)$ <u>or</u> $H'(\infty)$ within 0.2% or less, an error level comparable with the difference between $H_q(\infty)$ and $H'(\infty)$.

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*Careful numerical analysis of the Krook model shows that we would not be able, in the Monte Carlo calculations, to find at what time the quantity $[H_M(\tau) - H'(\infty)]$ becomes accurately proportional to $[t_q(0) - t_{\perp M}(\tau)]^2$, say within 2%, because of the smallness of these differences and the very gradual change of slope of the curves in the asymptotic region.

We may thus conclude that our Monte Carlo integration of the Boltzmann equation produces the correct asymptotic behavior of $t_\perp$ and H except for small errors that are to be expected from the nature of the numerical integrations over $\vec{v}$.

We may make a few remarks about the asymptotic statistical fluctuations of $t_{\perp M}(\tau)$ and of $H_M(\tau)$. The fluctuations of $t_{\perp M}$ (for $M > 0$) are roughly equal to the fluctuations in $t_{\perp M}$ found in Section 4.4 for an initial state of equilibrium ($M = 0$). The fluctuations of $H_M(\tau)$ (for $M > 0$), however, amount to about 0.01% for all Mach numbers and are therefore smaller by a factor of about five than were found for $M = 0$. Note that this remarkably small level of fluctuation was obtained with a rather small Monte Carlo sample, namely, $10^4$ collisions.

## 6.3. Behavior for $(t^{\frac{1}{2}}\tau) < 10$

### 6.31 $M \leq 6$

Two striking features of the curves in Figures 1 and 2 are evident for $M \leq 6$: they are almost straight and are nearly parallel. To discover how nearly straight and parallel we can say they are, we need to examine in detail various sources of error. We restrict our first discussion to the first ten steps in $\Delta\tau$ (for which $(t^{\frac{1}{2}}\tau) < 5$).

Data to permit estimation of the fluctuations in slope owing to the Monte Carlo calculations of the collision integral were obtained by the method described in Section 4.5. A typical "fan" generated by this method is shown in Figure 4. Since we were primarily interested in the apparent constancy of the slope as M changes we decided to examine first the mean slope and the (sample) standard deviation S for each set of four runs of ten intervals each. The slopes were determined by fitting a straight line (that passed through the

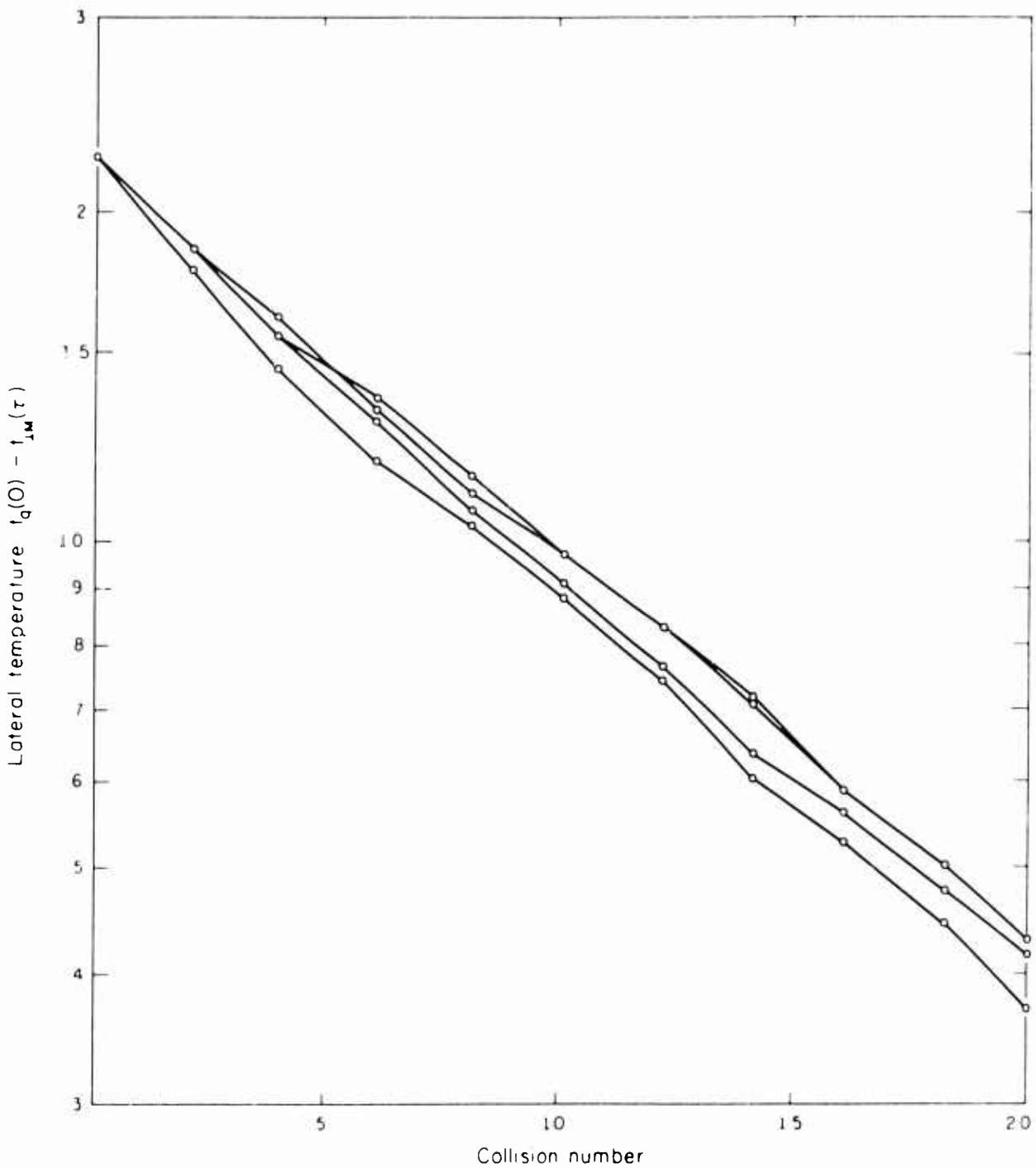


Figure 4. Temperature relaxation computed with four independent sequences of Monte Carlo samples. Each sample contains 10,923 collisions. Mach number M = 2.0.

point for $\tau = 0$) to the curve for each sample. The results are given in Table III and have been corrected for quadrature error in integrations with respect to $\tau$. (See Section 4.1.) It is unnecessary to correct for the difference between $t_a$ and $t_q(0)$ in the abscissa variable $(t^{\frac{1}{2}}\tau)$ because this difference is so small. (See Table II.)

Inspection shows that the variation among the mean slopes for the different Mach numbers is generally no larger than the 90% confidence limits for each Mach number. To make a more careful judgement we take the following steps:

a) Comparison of S - from variance ratio tests[13] we conclude that the sample standard deviations for the different Mach numbers are not significantly different at the 5% level.

b) Comparison of the means - an analysis of variations[13] shows that the sample means for the slopes of the H curves are not significantly different from one another at the 5% level. The mean slopes for $t_\perp$ agree with one another even better than do the mean slopes for H.

We may thus conclude that the logarithmic slopes of the relaxation curves (plotted vs $(t^{\frac{1}{2}}\tau)$) are independent of M for $t^{\frac{1}{2}}\tau \leq 5$ and $M \leq 6$, and are equal, respectively, to $0.3539 \pm 0.0122$ and $0.5607 \pm 0.0233$, the mean values of the slopes for $t_\perp$ and H. These values of mean slope and 90% confidence limits agree with values obtained less formally for the range $5 \leq (t^{\frac{1}{2}}\tau) \leq 10$. Detailed analysis in this range is less profitable because the estimated slopes are sensitive (for $(t^{\frac{1}{2}}\tau)$ near 10) to statistical fluctuations, to the exact choice of the nominal asymptotic values of the two variables, and to quadrature and truncation errors in integrations over $\vec{v}$.

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13. C. E. Weatherburn, A First Course in Mathematical Statistics (Cambridge 1961) Chap. X and XI.

Table III. Monte Carlo Fluctuations of Slope of Relaxation Curves

| | $t_\perp$ | | | H | | |
|---|---|---|---|---|---|---|
| M | mean slope | sample s.d. S | 90% confidence limits | mean slope | sample s.d. S | 90% confidence limits |
| 0.5 | .3598 | .0139 | .0189 | .5596 | .0338 | .0459 |
| 1.0 | .3451 | .0133 | .0180 | .6120 | .0197 | .0267 |
| 2.0 | .3536 | .0150 | .0203 | .5638 | .0268 | .0363 |
| 2.0* | .3528* | .0150* | .0203* | .5948* | .0268* | .0363* |
| 4.0 | .3599 | .0430 | .0583 | .5348 | .0842 | .1143 |
| 6.0 | .3522 | .0565 | .0767 | .4989 | .0708 | .0961 |
| mean | .3539 | | | .5607 | | |

*The starred values of mean slopes were obtained from one special run with a sample four times larger than any sample used for the other runs. For this special run we take the value of S and of the confidence limits to be the same as for the values given in the line above for the same Mach number M.

The analysis of the early part of the relaxation process has thus far dealt with the apparent parallelism of the curves, each curve having been assumed to be straight. We now ask, "How straight are the curves?" Inspection of the mean curves for each fan (and also the curves for the special large sample at M = 2.0) show no indication of curvature that cannot be attributed to statistical fluctuations or to small uncertainties in the choice of the asymptotic values of $t_q(0)$ and $H'(\infty)$.

Our over-all conclusions are that $t_\perp$ and H (for $M \lesssim 6$ and $(t^{\frac{1}{2}}\tau < 10)$ each relaxes as though it were governed by a single relaxation process.

$$t_\perp(\tau) = 1 + (t-1)\exp(-\beta_\perp t^{\frac{1}{2}}\tau) \tag{6-6}$$

$$H(\tau) = H(0) + [H(\infty) - H(0)]\exp(-\beta_H t^{\frac{1}{2}}\tau) \tag{6-7}$$

where

$$\beta_\perp = 0.3539 \pm 0.0122 \tag{6-8}$$

$$\beta_H = 0.5607 \pm 0.0233 \tag{6-9}$$

and are independent of M. The uncertainties are stated in terms of 90% confidence limits and are based upon observed Monte Carlo fluctuations. The uncertainties do not include estimates of possible systematic errors.

The ratio $\beta_H/\beta_\perp = 1.584 \pm 0.120$ (90% confidence limit) which, as predicted in Sect. 3, is somewhat smaller than the known asymptotic value of two.

Eq. (3-13) for the Krook model ($b_1 = b(0)$) corresponds to $\beta_\perp = \pi^{-1} = 0.318$. We may interpret the larger value, 0.354, obtained

by the Monte Carlo solution of the Boltzmann equation by finding for what molecular speed b(v) (for the equilibrium gas) is equal to $0.354\ t^{\frac{1}{2}}$. This speed is $0.51\bar{v}$ where $\bar{v}$ is the mean molecular speed. Molecules whose speed is less than $0.51\bar{v}$ relax more slowly than those whose speed is larger than $0.51\bar{v}$. This conclusion could be examined in detail by analysis of the time variation of the velocity distribution functions output in our calculations for each velocity bin.

The number of collisions in a reference gas necessary for relaxation by a factor of $e^{-1}$ is $\sqrt{2}/(\pi\beta) = 0.450/\beta$. The relaxation of $t_\perp$ and of H may then be described as follows: $1.27 \pm 0.044$ collisions of each molecule are required for relaxation of $t_\perp$ by the factor $e^{-1}$, and $0.80 \pm 0.033$ collisions are required for relaxation of H by the same factor. (The provisional value of this second number obtained by Alder and Wainwright[7] for a different starting condition was about one.) Each number is representative of the translational relaxation process initially and up to the time that relaxation by a factor of $e^{-2}$ or $e^{-3}$ has occurred. Asymptotically, only 0.64 collisions per molecule may be necessary for relaxation of H by the factor $e^{-1}$. (See Sect. 3.)

### 6.32 $M > 6$

For large enough values of M we should expect that the computational methods used here would break down. Errors then would enter because of the small number of velocity bins in which $f(\vec{v},0)$ is sensibly different from zero. The resulting quadrature errors amount to 29% and 5%, for n and t respectively, for M = 10. Even more serious quadrature errors arise in the Monte Carlo (or any other) numerical evaluation of the collision integral. In spite of these problems, $t_{\perp M}(\tau) \rightarrow t_q(0)$ and $H_M(\tau) \rightarrow H'(\infty)$ for M = 10 as $\tau$ increases. However, the behavior of $t_{\perp M}(\tau)$ and $H_M(\tau)$ for small times exhibits very large

fluctuations. We have not, therefore, presented our results in detail for $M = 10$.

It is possible that semi-analytical calculations like those of Alder and Wainwright[7] would give accurately the detailed pattern of translational relaxation for $M \gg 1$. Our methods could be used in relaxation calculations for values of $M > 6$ if we used a substantially larger number of velocity bins.