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ON THE ACCURACY OF APPROXIMATE SOLUTIONS OF THE BOLTZMANN EQUATION*

S.M. Yen and Bruce L. Hicks

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Abstract

Tests of the accuracy of approximate solutions of the Boltzmann equation for rarefied gas flow problems under conditions of strong deviation from thermal equilibrium have been developed by using the Nordsieck-Hicks Monte Carlo method of evaluating the collision integral. We have made and interpreted the tests for three approximate solutions for shock waves: Mott-Smith, 6-moment, and Navier-Stokes. In particular we have studied the collision integral for three approximate solutions, the distribution of errors of the solutions in velocity space, their relative inaccuracies at different positions in the shock, and certain moments of their distribution functions and collision integrals that are not calculable analytically.

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Introduction

Two methods have been described in the literature for obtaining approximate solutions of the Boltzmann equation for rarefied gas flow problems under conditions of strong deviation from thermal equilibrium: (1) finding velocity distributions whose lower order moments satisfy the Boltzmann transport equations; and (2) replacing the collision integral in the Boltzmann equation by an expression that approximates the integral and solving the resulting simpler "substitute" equation for the velocity distribution function. In the moment method only a limited number of properties of the distribution function are correct and they depend on arbitrarily chosen moments. As to the second method, the relation between either the microscopic or macroscopic properties calculated from the solutions of the substitute problem and those of the actual problem is not clear. Thus, for example, the representation of the collision integral by the BGK model for conditions far from thermal equilibrium is yet to be studied. Because of these uncertainties involved in the approximate solutions, the need for evaluating their accuracy has long been recognized.

There is no analytical solution of the Boltzmann equation for strong shocks. Attempts have been made to test the approximate solutions for a strong shock wave by examining the agreement between some macroscopic properties calculated from the solution, such as density and temperature profiles, and those determined by experiments; however, these comparisons give very little information concerning the accuracy of the approximate distribution functions. Agreement of such lower order moments is not an adequate measure of the departure of approximate solutions from exact solutions. Techniques have also been suggested for measuring directly the distribution functions, but such techniques have not been applied to flow within a shock wave. Even if we are able to check some of the pertinent properties of a theoretical shock against those determined by experiments, it would be of value to develop methods of studying in detail the accuracy of approximate solutions by evaluating the collision integral for these solutions. Such results would be directly useful in increasing the fidelity of the proposed approximate solutions.

Nordsieck and Hicks[1,2] have successfully developed a Monte Carlo method of evaluating the collision integral for any velocity distribution function and have applied it to a nonlinear translational relaxation problem and to the shock problem. We shall describe in this paper methods of testing approximate solutions of the Boltzmann equation for a strong shock wave that have been made possible by the development of the Monte Carlo method of evaluating the collision integral. Several different tests were made for the purpose of finding how well the approximate solutions satisfy the Boltzmann equation. Since we are able to calculate the collision integral for the approximate solutions, it is also possible to examine the distribution of the collision integral in the velocity space for each approximate solution. In addition, it is possible to evaluate the moments of the distribution function and those of the collision integral that cannot be obtained analytically. For example, we may determine whether the Boltzmann flux decreases monotonically in a shock wave.

We are able to test any approximate shock for hard sphere molecules with our computer program. We shall discuss in this paper detailed tests of three approximate solutions of the Boltzmann equation for a shock wave for several Mach numbers.

Methods of Testing Approximate Solutions

The Boltzmann equation for a shock wave may be written as

$$v_x(df/dx) = (a-bf) \tag{1}$$

in which $f = f(\bar{v},x)$ = velocity distribution function; $(a-bf)$ = collision integral (a = gain term, bf = loss term); v_x and $v_\perp$ are cylindrical polar coordinates in velocity space; and the x axis lies perpendicular to the plane of the shock wave.

We can first compute the collision integral for a given approximate solution $f^{(0)}$ by using the Monte Carlo method and then test how well the approximate solution satisfies the Boltzmann equation by using either of the following two tests:

(a) Test 1: comparing the calculated $(a-bf)^{(0)}$ with $v_x(df/dx)^{(0)}$ in the velocity space. (This test is equivalent to examining $\partial f/\partial t$.)

(b) Test 2: comparing in the velocity space each approximate solution $f^{(0)}$ with $f^{(1)}$, the next iterate, obtained by integrating the Boltzmann difference equation with respect to x.

If the Boltzmann equation were satisfied, then $(a-bf)^{(0)}$ would be equal to $v_x(df/dx)^{(0)}$ at each point in the velocity space and throughout the shock. Similarly, the f for any iteration, obtained by integrating the Boltzmann equation, would be the same as that for the previous iteration. Either test is sufficient to ascertain whether a given $f^{(0)}$ is the solution of the Boltzmann equation.

To obtain $f^{(1)}(\bar{v})$ at each station of a shock wave we perform a numerical integration of the following differential equation by a method developed by Nordsieck and Hicks:

$$v_x(df/dx)^{(1)} = (a-bf)^{(0)} \tag{2}$$

In our discussion we shall use the reduced number density

$$\hat{n} = (n - n_1)/(n_2 - n_1) \tag{3}$$

to identify the position in a shock wave.

Test 2, which requires determination of $f^{(1)}$, may be made for any distribution function after it is read into the computer memory by our program. On the other hand in Test 1 the determination of (df/dx) generally needs additional programming; however, for certain approximate shocks, like that of Mott-Smith, such programming is quite simple.

Since our Monte Carlo method evaluates the gain and loss terms (a and bf) of the collision integral separately, we are able to examine them separately for each approximate solution. Such results would be useful in studying the validity of any approximate model of the collision integral in which assumptions concerning both "b" and the ratio "a/b" are made.

For the approximate methods such as the moment method it is necessary to find explicit analytical formulae for the moments of both the distribution function and the collision integral. Such analytical calculations are sometimes quite tedious, and, indeed, some of the significant moments cannot be obtained analytically. We use the quadrature methods of Nordsieck and Hicks to calculate the following moments: $I_f(\phi)$ = moment of f, $I_A(\phi)$ = moment of a, and I_{AB} = moment of (a-bf) where ϕ = a function of molecular velocity. In our studies eleven functions were chosen for I_f and nine for I_A and I_{AB}. We note that the moment $I_{AB}(\phi)$ is equivalent to the gradient of the moment $I_f(\phi v_x)$. If ϕ is put equal to $1/v_x$ then the corresponding I_{AB} is equal to dn/dx, the density gradient. If $\phi = (1+\ln f)$ then the corresponding I_{AB} is the gradient of the Boltzmann flux.

Approximate Solutions Tested

As the first type of approximate solutions of the Boltzmann equation to be tested we chose the following bi-modal Ansatz for the distribution function:

$$f = f_\alpha + f_\beta \tag{4}$$

where $$f_\alpha = n_\alpha\,(m/2\pi kT_\alpha)^{3/2}\,\exp[-(m/2kT_\alpha)(\bar{v}-\bar{i}u_\alpha)^2] \tag{5}$$

$$f_\beta = n_\beta\,(m/2\pi kT_\beta)^{3/2}\,\exp[-(m/2kT_\beta)(\bar{v}-\bar{i}u_\beta)^2]$$

and n_α, n_β, T_α, T_β, u_α, and u_β are functions of x. We have tested two such approximate solutions: the Mott-Smith shock,[3] corresponding to the special case of constant T_α, T_β, u_α, and u_β; and the 6-moment shock,[4] corresponding to the general case of all six parameters variable. For the 6-moment method, in addition to three invariant moment equations, three moment equations corresponding to $\phi = v_x^2$, v_x^3, and $v_x v_\perp^2$ were used to obtain the solutions. The resulting macroscopic properties for Mach numbers near two indicate that the 6-moment shock represents a compromise between the Mott-Smith and Navier-Stokes shocks and shows improvements over the latter in the downstream region; however, the parameters T_α, T_β, u_α, and u_β vary significantly with $\hat{n}$ only near the upstream and downstream ends.

For the Mott-Smith distribution function, df/dn is constant and equal to $(f_2-f_1)/(n_2-n_1)$, and dn/dx, the density gradient, has the following simple quadratic form:

$$dn/dx = B(n-n_1)(n_2-n)/(n_2-n_1) \tag{6}$$

in which B is a constant to be determined by a chosen moment equation. We use the following functions in making the first test of the Mott-Smith shock:

$$L = (f_2-f_1)(n-n_1)(n_2-n)/(n_2-n_1) \tag{7}$$

$$Z = (a-bf)/v_x L \tag{8}$$

Since (a-bf) for the Mott-Smith shock has the same quadratic form as L, the ratio Z should be constant and equal to $B/(n_2-n_1)$ at each point in the velocity space and throughout the shock if the Mott-Smith shock satisfied the Boltzmann equation. Sakurai[5] has proved analytically that for large Mach numbers the ratio Z is constant for a finite velocity space. Recently, Oberai[6] has made similar investigations.

As a second type of approximate solution to be tested we chose the distribution functions corresponding to the Navier-Stokes shock.

Results and Discussion

We have made Test 2, that of comparing $f^{(1)}$ with $f^{(0)}$, for all three shocks; however, we have obtained results on Test 1 only for the Mott-Smith shock. We have chosen Monte Carlo sample sizes of approximately 131,000 to 700,000 collisions for Test 1, and 32,000 to 131,000 collisions for Test 2. Monte Carlo fluctuations were examined by using at least four statistically independent runs. The method[2] of improving the accuracy of the calculation of (a-bf) by forcing conservation of three moments has been used to obtain improved results. We shall discuss the results obtained both before and after this correction process.

For convenience of discussion we divide the finite velocity space[2] into three regions as shown schematically in Fig. 1. Region I is a semi-circle whose center and radius are determined by the Mach number. In most of this region df/dx and (a-bf) are negative. In region II, bounded by the line $v_x = 0$ and the boundary of region I, df/dx and (a-bf) are positive. In region III, for which v_x is negative, df/dx is positive and (a-bf) is negative. We therefore expect that (a-bf) vanishes at the boundary between regions II and III and near the boundary between regions I and II. These characteristics of the regions were deduced from various a priori arguments and were tested by calculating isoline plots for $(a\text{-}bf)v_\perp$ for a Mott-Smith shock with

$M = 1.5$, 2, 3, and 4 and a Monte Carlo sample of approximately 700,000 collisions. Inspection of the plots indicates that $(a-bf)v_{\perp}$ does have the characteristics described above.

The random and systematic errors in the evaluation of the collision integral have been studied carefully and are known to be small. For more accurate tests of the approximate solutions than those described here it will be necessary to extend our study of systematic errors.

In our calculations, the velocity space is divided into 226 velocity bins. For Test 2 the Boltzmann equation is integrated for each velocity bin to obtain $f^{(1)}$, which depends on the collision integrals for that velocity bin and therefore ultimately upon the values of $f^{(0)}$ for all bins.

(a) Results of Test 1:

We first compare the isoline plot of $(a-bf)v_{\perp}$ with the isoline plot of $(Lv_x)v_{\perp}$. Fig. 2 shows the two isoline plots at one position in a Mott-Smith shock for $M = 2$ and 4, obtained for a large Monte Carlo sample of approximately 700,000 collisions with no (a-bf) corrections. (The isoline plot of $(a-bf)v_{\perp}$ has the same form at any position in a Mott-Smith shock.) Although the two sets of isolines for each Mach number do have a considerable resemblance, the ratio of the values of the two functions, Z, varies considerably over velocity space as shown in Fig. 3. From these results it is quite evident that the Mott-Smith solution does not satisfy the Boltzmann equation <u>throughout the velocity space</u> for $M = 2$ and 4; however, for higher Mach numbers, the variation of the value Z was found to be small throughout a large part of region III. At the boundaries of regions I and II and regions II and III, the value Z has large fluctuations, since (a-bf) and Lv_x each becomes very small at these boundaries, and larger fractional errors are to be expected. If Z were very nearly constant in the velocity space, it might be compared with the value calculated by Mott-Smith for one of the arbitrarily chosen moment equations. For the moment equation with $\phi = v_x^2$ the calculated Mott-Smith value of Z in the same arbitrary units as used in Fig. 3 is 0.53 for $M = 2$ and 0.47 for $M = 4$.

We have also obtained improved results (by (a-bf) corrections) and analyzed the Monte Carlo fluctuations on the basis of these results. The contour-band plots of Z shown in Fig. 4 were obtained from results of four independent samples with a Monte Carlo sample of approximately 500,000 collisions. The width of the contour bands shows the Monte Carlo fluctuations among the four independent computer runs for the sample size used.

Results of Test 1 have also been obtained for $M = 6$, 8, and 10 for the Mott-Smith shock.

(b) Results of Test 2:

We choose to show contour intervals of the ratio $f^{(1)}/f^{(0)}$ for the second test. Fig. 5 shows these results with no (a-bf) corrections for three positions in a Mott-Smith shock and in a 6-moment shock for $M = 2$. Even though the parameters for the two shocks do not differ appreciably at the three locations chosen, the difference in the contours of the distribution function ratio is quite appreciable. In most parts of regions I and III for $\hat{n} = 1/4$ and $1/2$, $f^{(1)}/f^{(0)}$ is greater than one for the Mott-Smith shock and less than one for the 6-moment shock. Since $\int(a-bf)d\bar{v}$ (which is the mass flux) has the same value at each position in a shock wave, the existence of non-uniform distribution of $f^{(1)}/f^{(0)}$ is due to improper variation of the collision integral, corresponding to the approximate solution, over the velocity space.

The relative inaccuracy of an approximate shock in different regions of the velocity space may be found by examining the ratio of $f^{(1)}/f^{(0)}$ in these regions. For both Mott-Smith and 6-moment shocks, the ratio of $f^{(1)}/f^{(0)}$ lies between 0.95 and 1.05 for most regions at three chosen positions in a shock for $M = 2$ as shown in Fig. 5. The large deviation of $f^{(1)}/f^{(0)}$ from unity (greater than 1.05 and less than 0.95) occurs in the following domains of the velocity space for the Mott-Smith shock: (1) $\hat{n} = 1/4$ and $1/2$: the region with large speeds; (2) $\hat{n} = 3/4$: the region with large positive v_x and part of region I. In the 6-moment shock, similar deviations are found for positions corresponding to $\hat{n} = 1/4$ and $1/2$; however for $\hat{n} = 3/4$, the ratio $f^{(1)}/f^{(0)}$ is closer to unity in region I. The inaccuracy of both approximate solutions for fast molecules indicates that it may not be suitable to use these solutions for certain calculations such as those for ionization and dissociation. Fig. 6 shows the effect of Monte Carlo fluctuations evaluated from four runs with a sample size of approximately 131,000 collisions and corrections of (a-bf) to force conservation. In the regions where significant (a-bf) corrections were made, the ratio of $f^{(1)}/f^{(0)}$ is closer to one after the corrections were made. Studies of moments of (a-bf) seem to indicate that the corrections compensate for some bias of our Monte Carlo calculations. The regions corresponding to the different levels of $f^{(1)}/f^{(0)}$ remain qualitatively the same as before (a-bf) corrections.

We have also obtained results of the second test for Navier-Stokes shocks for M = 1.4, 1.6, 1.8 and 2.0. Fig. 7 shows these results for M = 1.4 and 2.0. We observe the following for M = 2: (1) the region at the periphery of the velocity space with positive v_x has a negative distribution function; (2) deviations of $f^{(1)}/f^{(0)}$ from unity that are much larger than those of either a Mott-Smith or a 6-moment shock occur in the region where molecular speeds are large at the position in the shock close to the cold side; (3) this region of very large deviations of $f^{(1)}/f^{(0)}$ becomes smaller for positions closer to the hot side. These results seem to support speculations made in the past that the Navier-Stokes shock is inaccurate near the upstream side of the shock. For M = 1.4, the ratio of $f^{(1)}/f^{(0)}$ in the greater part of the velocity space lies between 0.95 and 1.05 at the three positions in the shock considered. (We use a different scale of velocity for M = 1.4 in order to decrease quadrature error in calculating the collision integral.) Our results therefore confirm that the Navier-Stokes shock is more accurate at lower Mach numbers.

Another measure of the accuracy of the approximate solution is δf, the rms difference between $f^{(1)}$ and $f^{(0)}$. Values of δf for $M = 1.4$ to 2 are plotted in Fig. 8 for the Mott-Smith and Navier-Stokes shocks for $\hat{n} = 1/4$, 1/2, and 3/4. (The unit of n is n_1; the unit of velocity is $\sqrt{[2\pi k T_1/m]}$.) The large decrease in δf for the Navier-Stokes case when Mach number decreases again indicates that Navier-Stokes shock does have better accuracy at lower Mach numbers. The Mott-Smith shock is observed to have almost as good an accuracy, measured by δf, at $M = 2$ as at $M = 1.4$. However, the smallest values of δf shown in Fig. 8 for either approximation are more than 20 times as large as the residual errors in the Monte Carlo solution of the Boltzmann equation for fixed Monte Carlo samples.[2]

We also observe the following concerning the accuracy at different positions in these two shocks: for the Navier-Stokes shock, the position close to the hot side has better accuracy than the other two positions, while the position close to the cold side has better accuracy for the case of Mott-Smith shock.

(c) Numerical Calculations of Moments

As indicated earlier, we have calculated many moments of f, a, and (a-bf). We shall discuss two moments that cannot be evaluated analytically. Fig. 9 shows the behavior of the first of these two moments, the Boltzmann flux, for $M = 2$. We observe that all three shocks considered satisfy the condition that the Boltzmann flux decreases monotonically in a shock. The second interesting moment not calculable analytically is the function I_{AB} for $\phi = 1/v_x$.

This moment can be represented by B (see Eq. 6) and is plotted in Fig. 10 for a Mott-Smith shock as a function of M. For purposes of comparison, analytical calculations of B for <u>other</u> moments, represented by $\phi = v_x^2$, v_x^3, and $v_x v_\perp^2$, are also included in Fig. 10. It should be noted that I_{AB} for $\phi = 1/v_x$ is dn/dx for <u>any</u> shock, while only for the Mott-Smith shock are the other non-constant moments I_{AB} proportional to dn/dx. It is well known that Mott-Smith calculations do not give a unique value of B for dn/dx, and only I_{AB} for $\phi = v_x^2$ has been found to be in agreement with experimental results.[7] We observe from Fig. 10 that B for $\phi = 1/v_x$ agrees quite well with B for $\phi = v_x^2$.

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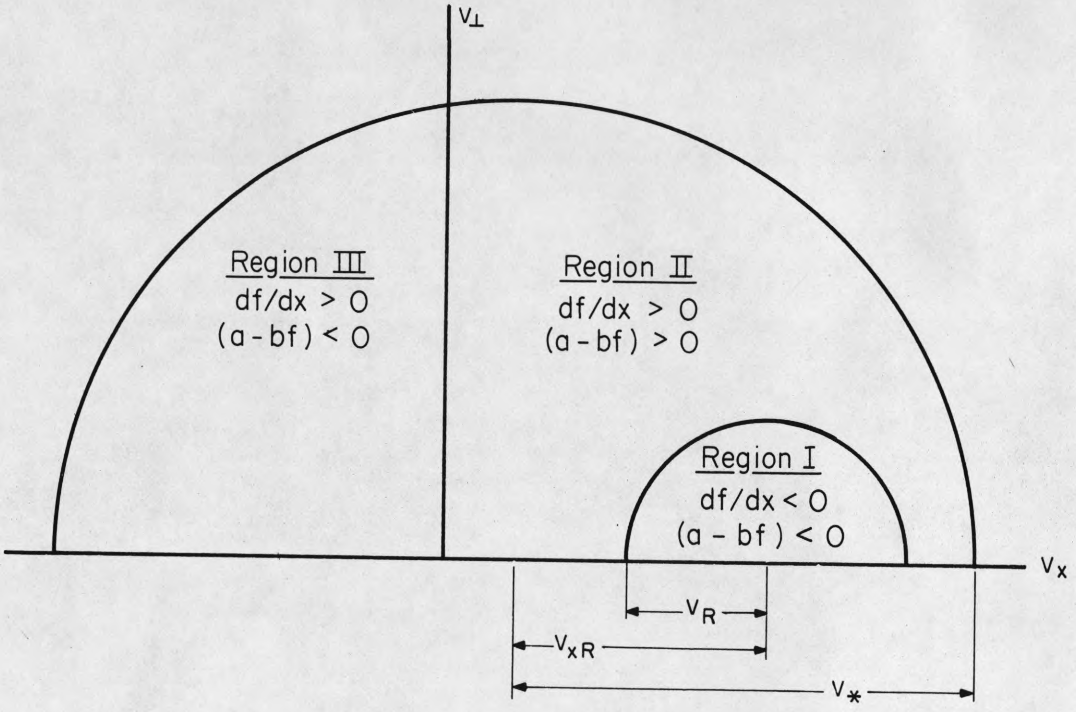


v_x and $v_\perp$ are cylindrical polar coordinates

Fig. 1 Finite velocity space considered and expected signs of df/dx and (a-bf) in different regions.

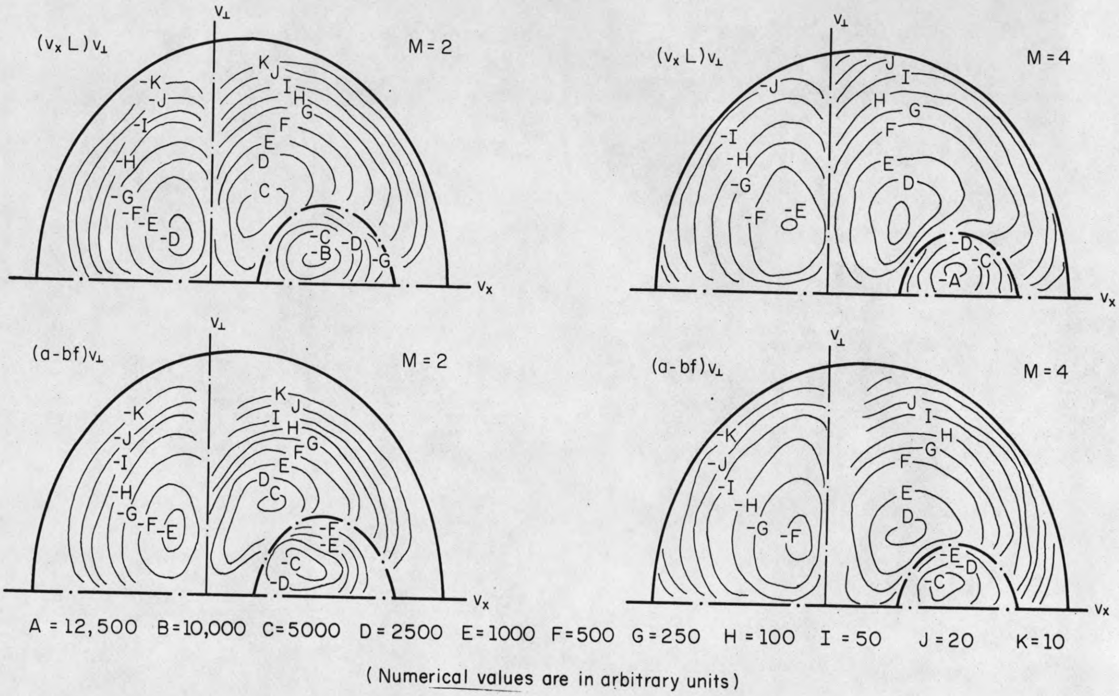


Fig. 2 Isolines of the collision integrals $(a-bf)v_\perp$ and $(Lv_x)v_\perp$ for Mott-Smith shock of M = 2 and 4. $L = (f_2-f_1)(n_2-n)(n-n_1)/(n_2-n_1)$. Monte Carlo sample = 700,000 collisions approximately. No $(a-bf)^{(0)}$ corrections.

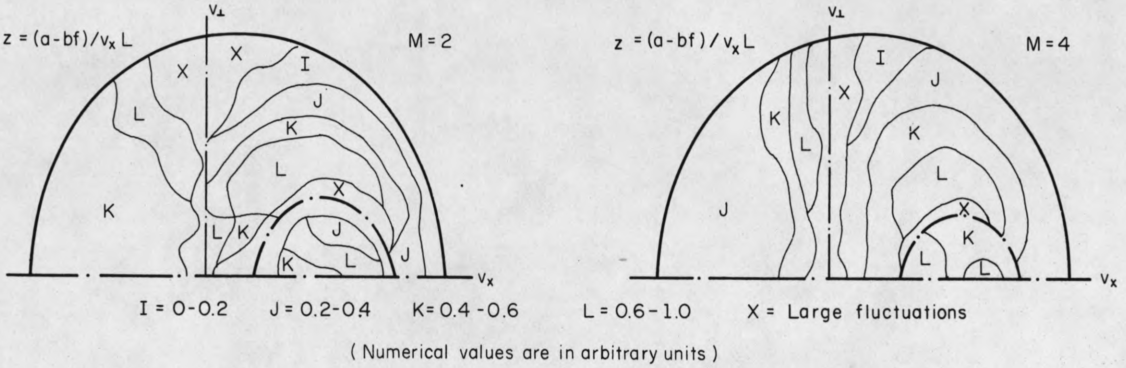


Fig. 3 Contour interval plot of Z in arbitrary units for Mott-Smith shock of M = 2 and 4. Values of Z correspond to the results given in Fig. 2.

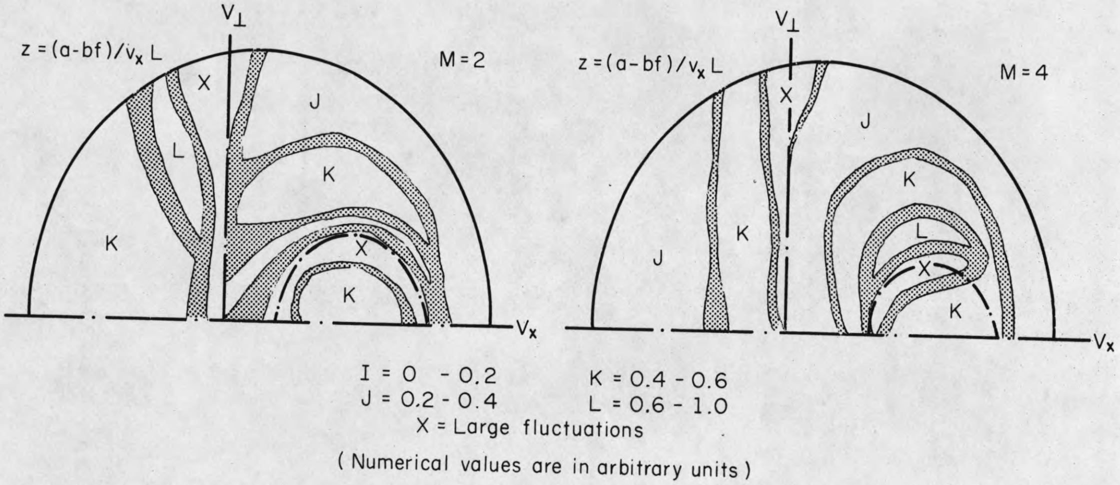
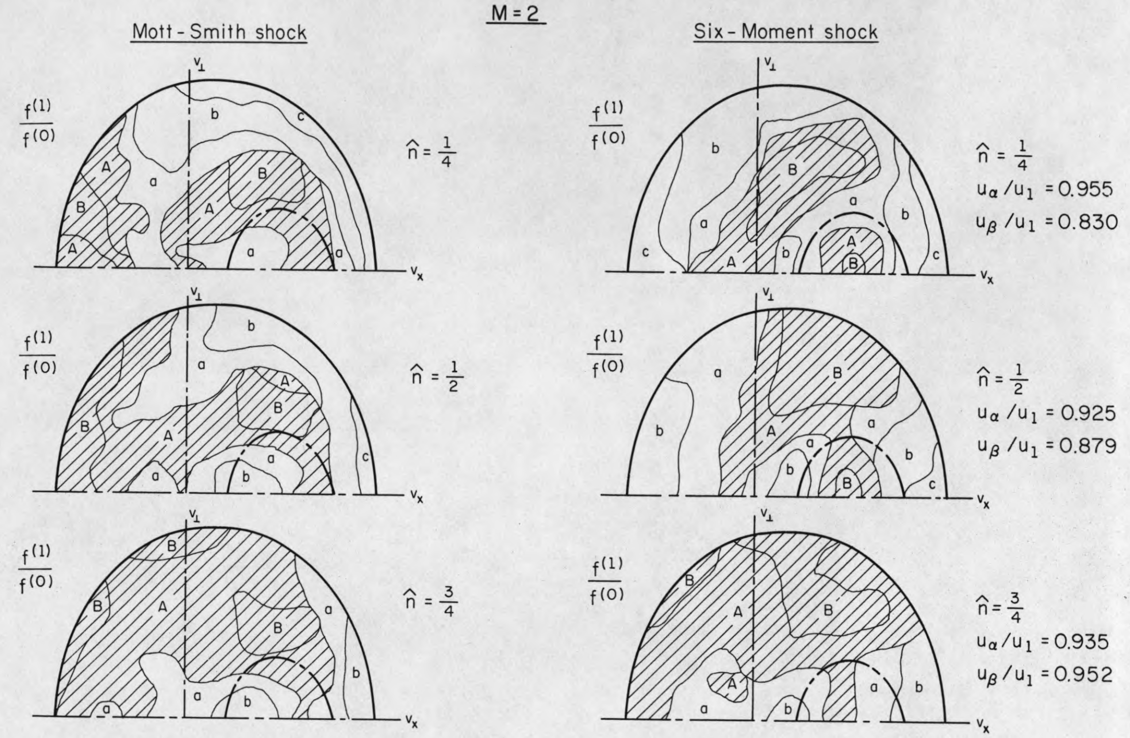


Fig. 4 Contour-band plot of Z in arbitrary units for Mott-Smith shock of M = 2 and 4. Results were obtained from four computer runs of independent collision samples (sample size = 2^{19}).



$\hat{n} = (n-n_1)/(n_2-n_1)$

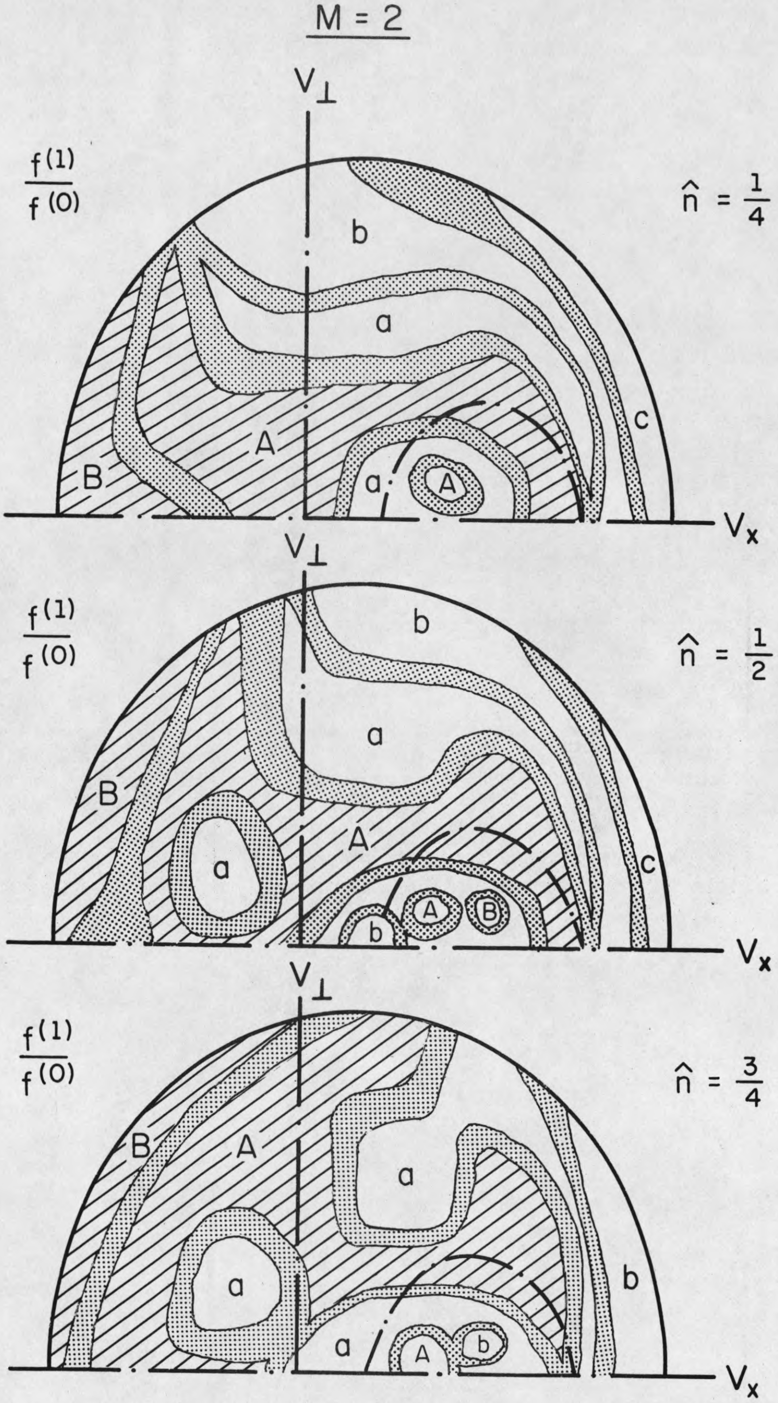
Cross-hatched regions: $f^{(1)} > f^{(0)}$

c = 0.60-0.80, b = 0.80-0.95, a = 0.95-1.00

A = 1.00-1.05, B = 1.05-1.20

(Numerical values in arbitrary units)

Fig. 5 Contour interval plot of the ratio $f^{(1)}/f^{(0)}$ at three positions in a Mott-Smith shock and a 6-moment shock. M = 2. $(a-bf)^{(0)}$ used was calculated with a Monte Carlo sample of 2^{17} collisions. $(a-bf)^{(0)}$ was not corrected.



$\hat{n} = (n - n_1)/(n_2 - n_1)$

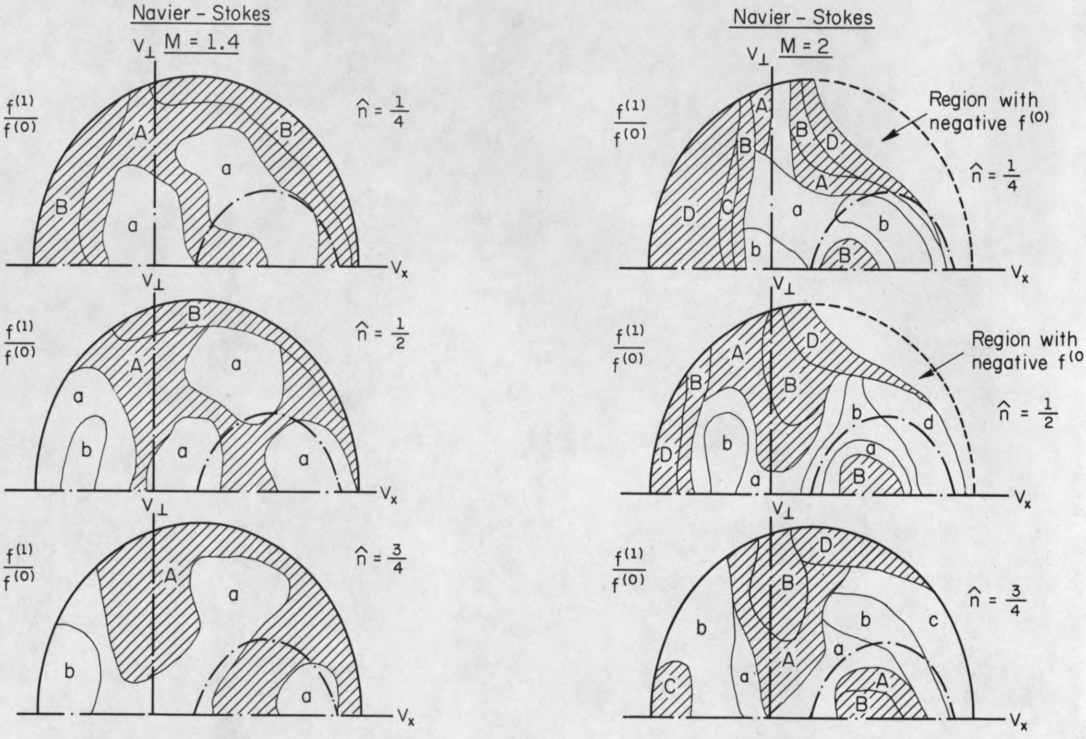
Cross-hatched regions: $f^{(1)} > f^{(0)}$

c = 0.60 - 0.80, b = 0.80 - 0.95, a = 0.95 - 1.00

A = 1.00 - 1.05, B = 1.05 - 1.20

(Numerical values are in arbitrary units)

Fig. 6 Contour-band plot of the ratio $f^{(1)}/f^{(0)}$ at three positions in a Mott-Smith shock. The results were obtained with four computer runs of independent samples (sample size = 2^{17} collisions) and with $(a-bf)^{(0)}$ corrections.



$\hat{n} = (n-n_1)/(n_2-n_1)$

Cross-hatched regions: $f^{(1)} > f^{(0)}$

c = 0.60 - 0.80, b = 0.80 - 0.95, a = 0.95 - 1.00

A = 1.00 - 1.05, B = 1.05 - 1.20, C = 1.20 - 1.70, D = 1.70 - 6.00

(Numerical values are in arbitrary units)

Fig. 7 Contour interval plot of the ratio $f^{(1)}/f^{(0)}$ at three positions in a Navier-Stokes shock. M = 1.4 and 2. $(a-bf)^{(0)}$ used was calculated with a Monte Carlo sample of 2^{17} collisions. $(a-bf)^{(0)}$ was corrected.

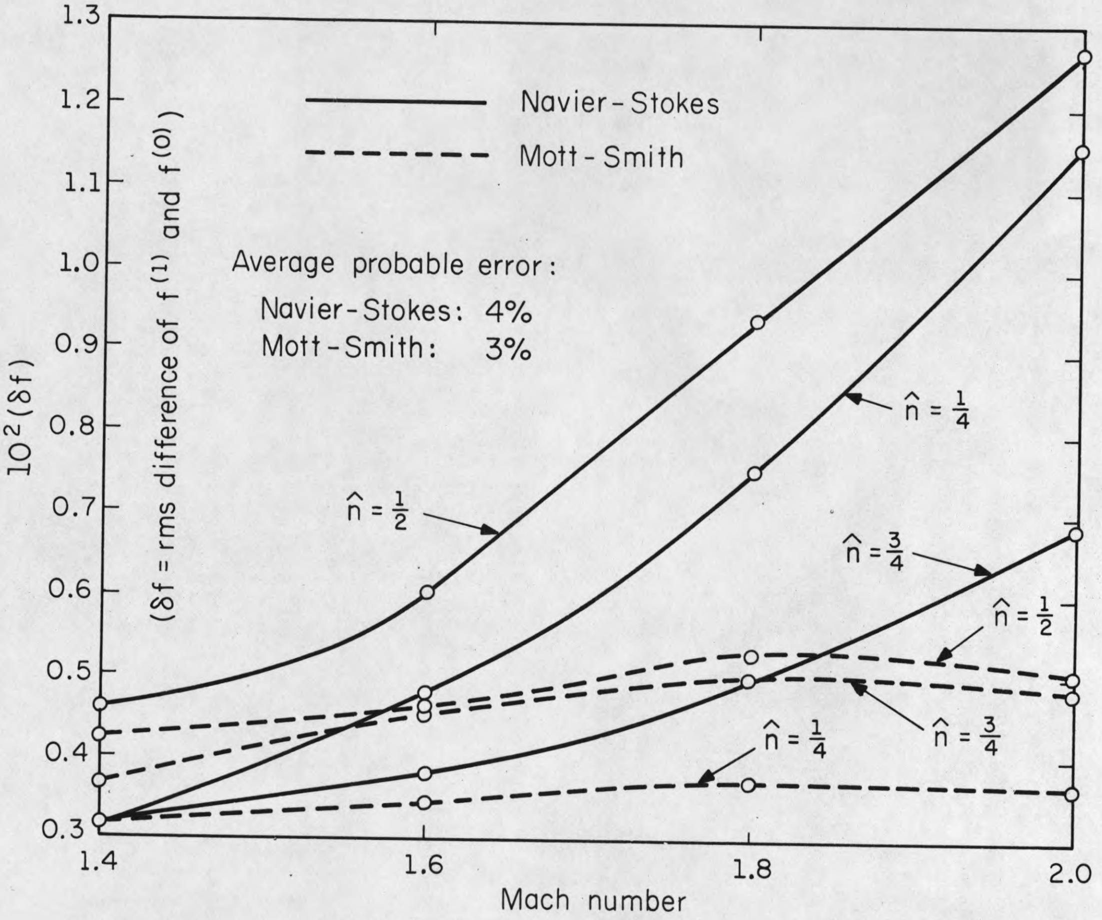


Fig. 8 Variation of δf, rms difference between $f^{(0)}$ and $f^{(1)}$, at three positions in Mott-Smith and Navier-Stokes shocks, plotted vs Mach number.

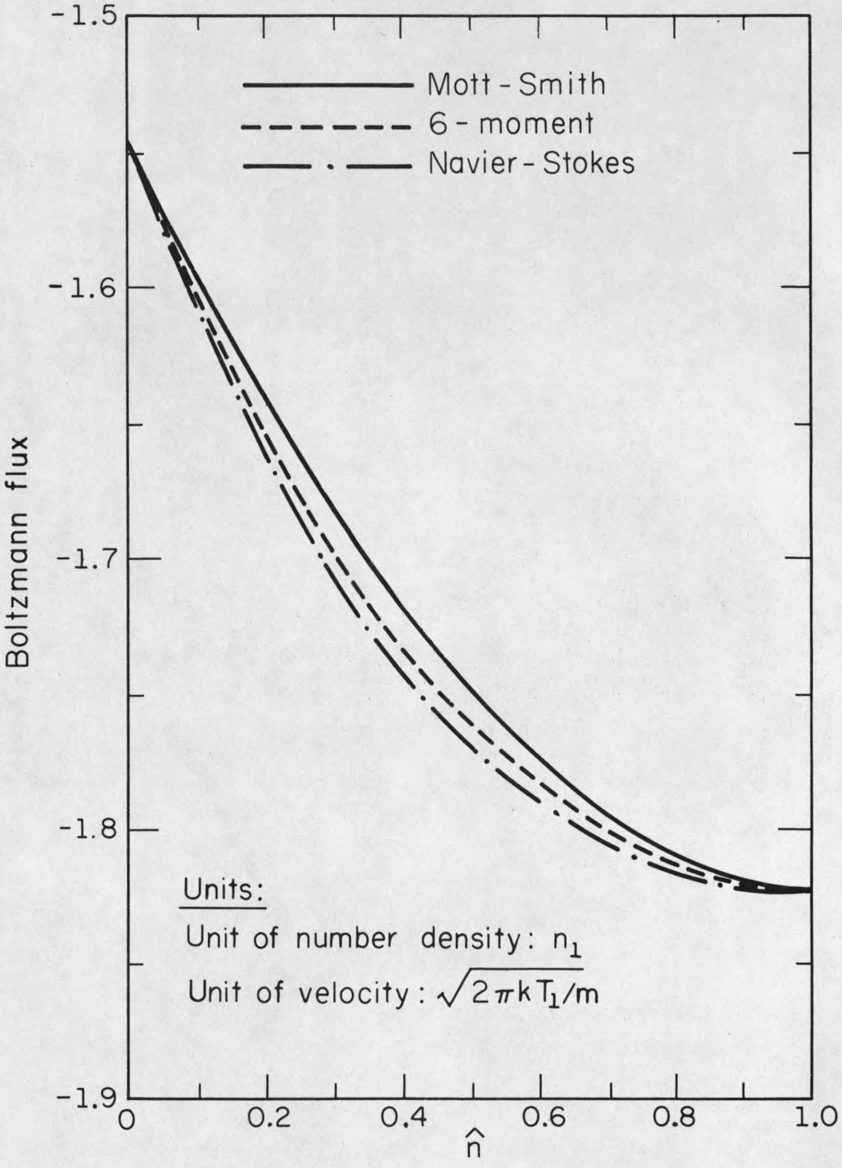


Fig. 9 Variation of Boltzmann flux with $\hat{n}$ for M = 2.

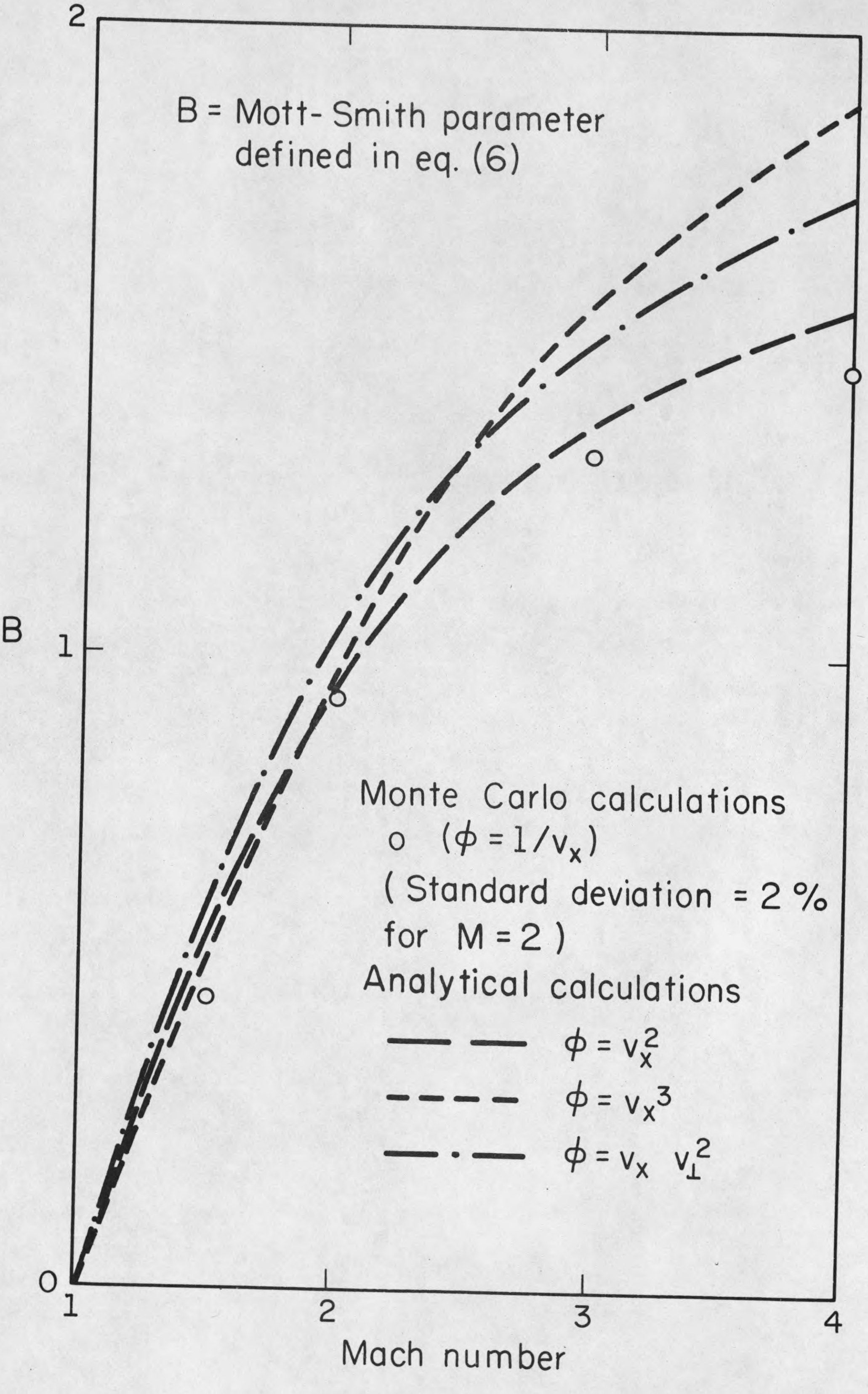


Fig. 10 Variation of B with Mach number.

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