Iterative method to improve the Mott-Smith shock-wave structure theory

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In order to improve the Mott-Smith theory for shock-wave structures, an iterative method is introduced. The method is basically one of the family of iterative schemes constructed by Ikenberry and Truesdell [J. Rat. Mech. Anal. **5**, 1 (1956)]. In the present work, the initial values for the iteration are calculated by using the Mott-Smith bimodal function [Phys. Rev. **82**, 885 (1951)]; the equilibrium Maxwellian function is used in conventional Ikenberry-Truesdell–type approaches. The density profile in the first iterative step for monatomic Maxwellian molecular gases has been obtained in a closed form. Within the limitation of the lowest-order calculation, the results show asymmetric density profiles, the correct shock thickness limiting law at the weak limit, and nonmonotonic kinetic temperature profiles even for monatomic molecules.
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I. INTRODUCTION

During the past half century much research has addressed the shock-wave structure problem using the pioneering work of Mott-Smith. Mott-Smith [1] pointed out that the distribution function of molecular velocities in a strong shock wave in a gas is bimodal. This can be rewritten as

$$f_{\mathrm{MS}}(\mathbf{v},x)=\nu(x)f_{\mathrm{M}}^{(u)}(\mathbf{v})+[1-\nu(x)]f_{\mathrm{M}}^{(d)}(\mathbf{v}), \tag{1}$$

where $f_{\mathrm{M}}^{(u)}(\mathbf{v})$ and $f_{\mathrm{M}}^{(d)}(\mathbf{v})$ are the upstream and downstream Maxwellian distribution functions, respectively, and $\nu(x)$ is the unknown quantity obtained from the Boltzmann equation. The Monte Carlo experiments and the direct numerical analyses of the Boltzmann equation indicate that the bimodal function represents the actual velocity distribution of molecules quite well in strong shock layers [2]. Because of its remarkable simplicity and its correct predictions in strong-shock-wave experiments, the Mott-Smith theory has been applied to a wide area of shock phenomena [3,4] including the shock structures of dense gases [5] and relativistic shocks [6]. However, there are two nontrivial deficiencies in the theory. The first is the lack of a unique way to determine the unknown quantity $\nu(x)$. Usually the $\nu(x)$ is determined from a moment equation given by the Boltzmann equation. The choice of velocity moment is to an extent arbitrary, but the result depends markedly on this choice [7]. The second deficiency is the incorrect shock thickness limiting law at a weak shock. Since the Navier-Stokes theory is believed to be exact at the weak shock limit, the discrepancy between the Mott-Smith and the Navier-Stokes limiting laws has been noted and the former deemed incorrect [8].

Although different approaches have attempted to improve the Mott-Smith theory [9–14], we propose an alternative method to eliminate both deficiencies of the Mott-Smith theory [15]. Our method is based on the iterative approach first used by Maxwell and later systematically developed by Ikenberry and Truesdell [16,17]. The Maxwell-Ikenberry-Truesdell (MIT) approach employs the Maxwellian distribution function for the initial values in beginning the iteration. In the present work, we use the Mott-Smith bimodal distribution function to calculate these values and follow the MIT iteration procedure, restricting ourselves to the first iteration for monatomic Maxwellian molecules.

II. FORMULATION OF SHOCK-WAVE PROBLEM

It is customary to start by writing down the hydrodynamic equations for the one-dimensional steady state

$$\frac{d}{dx}(\rho u_x)=0, \tag{2a}$$

$$\rho u_x\frac{du_x}{dx}+\frac{d}{dx}(\Pi_{xx}+p)=0, \tag{2b}$$

$$\rho u_x\frac{d\mathcal{E}}{dx}+\frac{dQ_x}{dx}+(\Pi_{xx}+p)\frac{du_x}{dx}=0, \tag{2c}$$

where ρ is the mass density, u_x the streaming velocity, Π_{xx} the normal viscous stress, p the pressure, $\mathcal{E}$ the internal energy density, and Q_x the heat flux. For monatomic dilute gases, $\mathcal{E}$ is related to the kinetic temperature T by $d\mathcal{E}/dx=c_v dT/dx$ in which $c_v=\frac{3}{2}k_{\mathrm{B}}/m$ with the Boltzmann constant k_{B} and the molecular mass m.

Integrating both sides of Eqs. (2) from $x=-\infty$ (equilibrium upstream by definition) to a certain x, one obtains

$$\rho u_x=\rho^{(u)}u_x^{(u)}, \tag{3a}$$

$$\rho u_x^2+\Pi_{xx}+p=\rho^{(u)}(u_x^{(u)})^2+p^{(u)}, \tag{3b}$$

$$\rho u_x c_v T+Q_x+(\Pi_{xx}+p)u_x+\tfrac{1}{2}\rho u_x^3 = \rho^{(u)}u_x^{(u)}c_v T^{(u)}+u_x^{(u)}p^{(u)}+\tfrac{1}{2}\rho^{(u)}(u_x^{(u)})^3, \tag{3c}$$

in which the superscript (u) denotes the quantity of the upstream. It is convenient to introduce the dimensionless quantities

$$\tilde{\rho}\equiv\rho/\rho^{(u)},\quad \tilde{u}\equiv u_x/u_x^{(u)},\quad \tilde{T}\equiv T/T^{(u)},$$

$$\tilde{p}\equiv p/\rho^{(u)}(u_x^{(u)})^2, \quad \tilde{\Pi}\equiv \Pi_{xx}/\rho^{(u)}(u_x^{(u)})^2,$$

$$\tilde{Q}\equiv Q_x/\rho^{(u)}(u_x^{(u)})^3, \quad B\equiv k_B T^{(u)}/m(u_x^{(u)})^2.$$

Since $\tilde{p}=B\tilde{\rho}\tilde{T}$, Eqs. (3) are rewritten as

$$\tilde{\rho}\tilde{u}=1, \tag{4a}$$

$$\tilde{u}+\tilde{\Pi}+B\tilde{\rho}\tilde{T}=1+B, \tag{4b}$$

$$5B\tilde{T}+2\tilde{Q}+2\tilde{u}\tilde{\Pi}+\tilde{u}^2=1+5B. \tag{4c}$$

The parameter B is related to the Mach number of the upstream velocity M through

$$M\equiv u_x^{(u)}/U_s=\left(\frac{3}{5B}\right)^{1/2}, \tag{5}$$

where U_s is the sound speed in the upstream, which is equal to $(5k_BT^{(u)}/3m)^{1/2}$ for monatomic dilute gases [8]. The equilibrium values in the upstream and downstream are immediately obtained by solving Eqs. (4) simultaneously because both $\tilde{\Pi}$ and $\tilde{Q}$ vanish. In order to have the values in the shock layer, however, one has to know about the nonvanishing $\tilde{\Pi}$ and $\tilde{Q}$, which are to be calculated by the iterative method.

III. THE MIT ITERATION

Ikenberry and Truesdell [16,17] constructed a family of iterative methods that extracts with successive approximations the mathematical relations between the physical quantities of gases from the Boltzmann equation. One member of the family they called the ''Maxwell iteration'' constitutes the basic method, which we will follow in this paper. We can start by writing down the one-dimensional moment equations for Π_{xx} and Q_x,

$$\frac{dR^{(3)}}{dx}-\frac{2}{3}\frac{dQ_x}{dx}+u_x\frac{d\Pi_{xx}}{dx}+\frac{1}{3}(7\Pi_{xx}+4p)\frac{du_x}{dx}=\Lambda^{(\Pi)}, \tag{6a}$$

$$\frac{dR^{(4)}}{dx}+2u_x\frac{dQ_x}{dx}-\frac{1}{\rho}(2\Pi_{xx}+5p)\frac{d}{dx}(\Pi_{xx}+p)+2(R^{(3)}+2Q_x)\frac{du_x}{dx}=\Lambda^{(Q)}. \tag{6b}$$

The moments in Eqs. (6) are defined by the velocity distribution function in the kinetic theory of gases as

$$p=\int \frac{1}{3}mC^2 f d\mathbf{C}, \tag{7a}$$

$$\Pi_{xx}=\int m(C_x^2-\tfrac{1}{3}C^2)f d\mathbf{C}, \tag{7b}$$

$$Q_x=\int \frac{1}{2}mC_xC^2 f d\mathbf{C}, \tag{7c}$$

$$R^{(3)}=\int mC_x^3 f d\mathbf{C}, \tag{7d}$$

$$R^{(4)}=\int mC_x^2C^2 f d\mathbf{C}, \tag{7e}$$

in which $\mathbf{C}$ is the peculiar velocity of molecules. $\Lambda^{(\Pi)}$ and $\Lambda^{(Q)}$ in Eqs. (6) are derived from the collision integral of the Boltzmann equation. As for the monatomic Maxwellian molecules [17], these are written as

$$\Lambda^{(\Pi)}=-\frac{p}{\eta}\Pi_{xx}, \tag{8a}$$

$$\Lambda^{(Q)}=-\frac{4p}{3\eta}Q_x, \tag{8b}$$

where η is the viscosity. In the MIT iteration scheme, one calculates the new right-hand-sides values (the collision terms) using the old left-hand sides (the streaming terms) in Eqs. (6). One needs the equations of $R^{(3)}$ and $R^{(4)}$ for the second iteration and more equations for higher step iterations. Using the dimensionless quantities, Eqs. (6) are rewritten in iterative form

$$\frac{d\tilde{R}_{[r]}^{(3)}}{d\tilde{x}}-\frac{2}{3}\frac{d\tilde{Q}_{[r]}}{d\tilde{x}}+\tilde{u}\frac{d\tilde{\Pi}_{[r]}}{d\tilde{x}}+\frac{1}{3}(7\tilde{\Pi}_{[r]}+4\tilde{p}_{[r]})\frac{d\tilde{u}}{d\tilde{x}}=-\frac{8}{5}\left(\frac{2B}{\pi}\right)^{1/2}\tilde{\rho}\tilde{\Pi}_{[r+1]}, \tag{9a}$$

$$\frac{d\tilde{R}_{[r]}^{(4)}}{d\tilde{x}}+2\tilde{u}\frac{d\tilde{Q}_{[r]}}{d\tilde{x}}-\frac{1}{\rho}(2\tilde{\Pi}_{[r]}+5\tilde{p}_{[r]})\frac{d}{d\tilde{x}}(\tilde{\Pi}_{[r]}+\tilde{p}_{[r]})+2(\tilde{R}_{[r]}^{(3)}+2\tilde{Q}_{[r]})\frac{d\tilde{u}}{d\tilde{x}}=-\frac{32}{15}\left(\frac{2B}{\pi}\right)^{1/2}\tilde{\rho}\tilde{Q}_{[r+1]} \tag{9b}$$

for the $(r+1)$th iteration, where $\tilde{x}$ is the reduced distance scaled by the upstream mean free path λ, which is an effective free path [8] established by substituting the theoretical viscosity of the Maxwellian molecules into a hard-sphere relationship between the mean free path and the viscosity; $\tilde{R}^{(3)}\equiv R^{(3)}/\rho(u_x^{(u)})^3$ and $\tilde{R}^{(4)}\equiv R^{(4)}/\rho(u_x^{(u)})^4$.

The first iteration corresponds to the lowest-order calculation that $r=0$ in Eqs. (9). The initial values for the iteration are calculated by the definitions of velocity moments given in Eqs. (7) with the help of the bimodal distribution function. Since the bimodal function has only one unknown quantity ν, all the initial values in the streaming terms of Eqs. (9) are expressed in its functionals. Without any difficulties, the independent variable can be changed from ν to $\tilde{\rho}$. After some algebraic manipulations, one obtains the first iterates as

$$\frac{1}{8}(1+5B)(1+B)\frac{d\tilde{\rho}}{d\tilde{x}}=\frac{8}{5}\left(\frac{2B}{\pi}\right)^{1/2}\tilde{\rho}\tilde{\Pi}_{[1]}, \tag{10a}$$

$$\frac{1+5B}{32\widetilde{\rho}}[\widetilde{\rho}(1-10B+5B^2)+8(1+B)]\frac{d\widetilde{\rho}}{d\widetilde{x}} = -\frac{32}{15}\left(\frac{2B}{\pi}\right)^{1/2}\widetilde{\rho}\widetilde{Q}_{[1]}. \tag{10b}$$

The first iteration implies that the streaming terms in Eqs. (9) are approximated by the values of the bimodal distribution function to find the unknown collision terms. The obtained values $\widetilde{\Pi}_{[1]}$ and $\widetilde{Q}_{[1]}$ are used in the hydrodynamic equations (4) to get the shock profiles. After some rearranging, we have the equation

$$\frac{d\widetilde{\rho}}{d\widetilde{x}}=\frac{512}{15}\left(\frac{2B}{\pi}\right)^{1/2}\frac{(\widetilde{\rho}-1)(4-5B\widetilde{\rho}-\widetilde{\rho})}{(1+5B)[\widetilde{\rho}(1-10B+5B^2)+16(1+B)]}. \tag{11}$$

Let us define a normalized density

$$\rho^*\equiv(\rho-\rho^{(u)})/(\rho^{(d)}-\rho^{(u)})$$

and take the origin $x=0$ as the point where $\rho^*=\frac{1}{2}$. Then the solution of Eq. (11) is written as

$$\rho^*/(1-\rho^*)^{a+1}=2^a\exp(b\widetilde{x}), \tag{12}$$

where

$$a=\frac{(3-5B)(1-10B+5B^2)}{(1+5B)(17+6B+5B^2)} \tag{13}$$

and

$$b=\frac{512}{15}\left(\frac{2B}{\pi}\right)^{1/2}\frac{3-5B}{(1+5B)(17+6B+5B^2)}. \tag{14}$$

Equation (12) is the main result of the present study. The profiles of the other quantities are obtained from Eqs. (4) and (10) with the use of Eq. (12).

IV. DISCUSSION

It should be noticed that the density profile shape given by Eq. (12) is asymmetric. It has been argued that the symmetric density profile from the original Mott-Smith theory is a defect in the theory because experimental density profiles are asymmetric for all Mach numbers [18]. The shock thickness Δ is defined by using the maximum density slope as

$$\Delta\equiv(\rho^{(d)}-\rho^{(u)})\Big/\left|\frac{d\rho}{dx}\right|_{\max}$$

and the dimensionless reciprocal thickness λ/Δ is a parameter that is used for comparing calculations to experiments. Since B in Eqs. (13) and (14) is related to the Mach number through Eq. (5), the limiting properties of the shock profiles are evaluated immediately. For $M\to1$, the reciprocal thickness takes the form

$$\lambda/\Delta_{\text{weak}}=\frac{4}{7}\left(\frac{6}{5\pi}\right)^{1/2}(M-1),$$

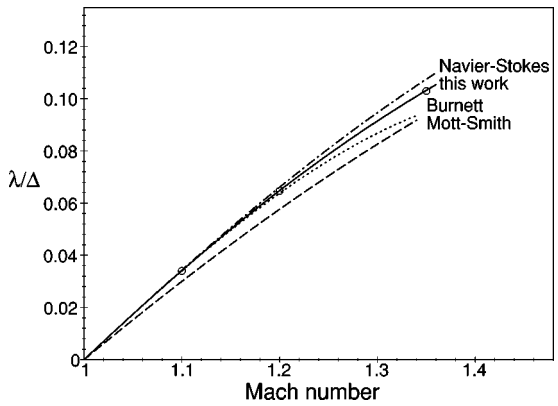

FIG. 1. Dimensionless reciprocal density thickness of weak shock waves. The curves for Navier-Stokes and Burnett theories are the values of Chang [8]. ○ denotes the Monte Carlo result [19].

which is in exact accord with the Navier-Stokes theory [8].

In order to compare the results of this work with the values for the Maxwellian molecules in the literature, the reciprocal density thicknesses are illustrated in Figs. 1 and 2. For weak shocks of $M<1.5$, agreement between the first iterative calculations and the Monte Carlo experiments [19] is excellent, giving the correct limiting law. For strong shocks of $M>2$, the present work underestimates by about 30% the Monte Carlo results [20,21], which are even worse than the Mott-Smith v_x^2 choice [22]. This discrepancy is regarded as a limitation of the lowest-order iteration, which is reduced by the higher-order iterations. In Fig. 3 the normalized density profiles are compared with the calculations of the Mott-Smith v_x^2 choice. The density profile shows a monotonic increase from upstream to downstream. The kinetic temperature profile, however, shows the maximum point within the shock layer, which is absent in the Mott-Smith theory [23]. The nonmonotonic profile occurs when $M>3.313$. It is well known that this kind of temperature profile is not a mathematical artifact but the result of atomistic dynamics [2,21,24,25]. The profiles of normalized kinetic temperatures are compared in Fig. 4 with the Mott-Smith calculation, where the normalized kinetic temperature is defined as

$$T^*\equiv(T-T^{(u)})/(T^{(d)}-T^{(u)}).$$

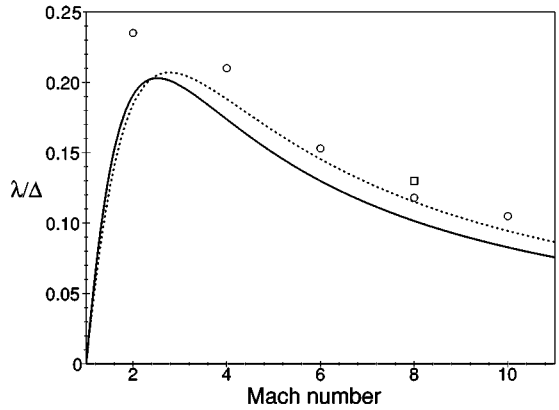

FIG. 2. Dimensionless reciprocal density thickness of strong shock waves. —, this work; · · ·, the Mott-Smith v_x^2 choice; ○, the Monte Carlo result of Yen and Ng [20]; □, the Monte Carlo result of Bird [21].

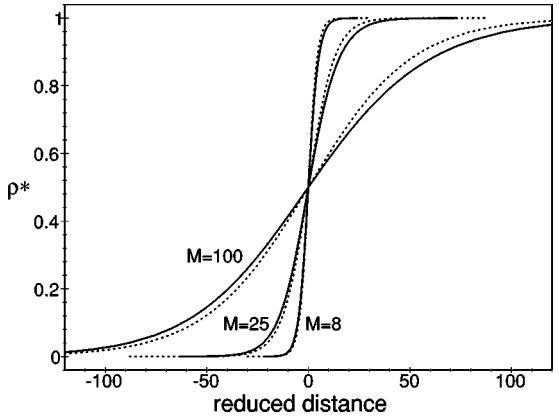

FIG. 3. Normalized density profiles vs reduced distance (x/λ). —, this work; ⋯, the Mott-Smith v_x^2 choice.

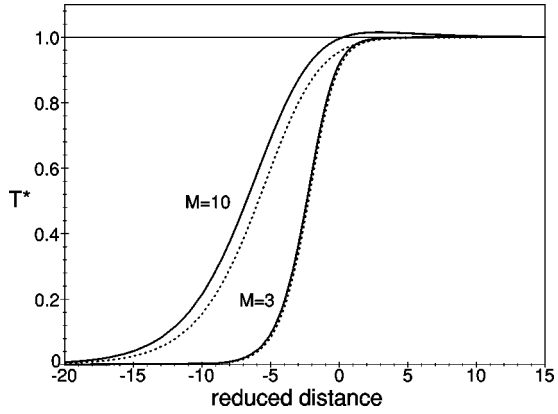

FIG. 4. Normalized kinetic temperature profiles vs reduced distance (x/λ). —, this work; ⋯, the Mott-Smith v_x^2 choice.

V. CONCLUSION

In conclusion, the Mott-Smith theory can be systematically improved by introducing an iterative scheme for the calculations of unknown moments. At the lowest iterative step, the evidence of improvement is clear. Following the suggestions of Ikenberry and Truesdell, there is a variety of iterative methods [16]. The other iterative methods will give similar results as long as the initial values are calculated using the Mott-Smith bimodal distribution function. The variety of iterative methods does not indicate the lack of a unique way to determine the unknown moments such as in the original Mott-Smith theory. The choice of iterative method depends mainly on the convergence, which will at last give the exact result.

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