Generalized hydrodynamic theory of shock waves in rigid diatomic gases

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Generalized hydrodynamic theory of shock waves is phenomenologically developed for rigid diatomic molecules. The generalized hydrodynamic equations developed are thermodynamically consistent, obeying the laws of thermodynamics. They reduce to the Navier-Stokes-Fourier theory of the classical hydrodynamics in the limit of low Mach number. The theory is applied to study the one-dimensional shock wave structure of nitrogen gas, which is treated as a rigid molecule. An excellent agreement with experiment is obtained for the inverse shock widths up to Mach number 10 reported in the literature. The theory is applicable to arbitrary dimension. On the basis of direction field singularities of the velocity and temperature evolution equations of the theory, it is possible to predict that the shock solutions exist for all Mach numbers in the case of one-dimensional shock waves studied.

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I. INTRODUCTION

Shock wave structures of monatomic and molecular gases are not only interesting and important from the technological viewpoint, but also serve as an important and sensitive touchstone for the ability of continuum hydrodynamic equations to describe macroscopic phenomena in the substances mentioned. It is well known that the Navier-Stokes-Fourier (NSF) equations of the classical hydrodynamics are incapable of accurately describing shock wave phenomena in both monatomic and molecular fluids in the hypersonic regime and also flow phenomena in rarefied gases. It has remained an outstanding problem in fluid dynamics to extend [1–11] the classical theory so as to make the continuum mechanics approach serviceable to the shock wave phenomena in the regime of hypersonic speed and also to rarefied gas dynamics phenomena [12,13] in the large Knudsen number regime. In fact, the voluminous literature in gas dynamics and fluid mechanics that deals with theories beyond the classical hydrodynamic method by using simulation methods of one kind or another is in a sense the witness to the failure of the classical hydrodynamics. The lacuna left by the unanswered challenges in the continuum mechanics approach has been mostly filled by computer simulation methods, notably, the direct simulation Monte Carlo (DSMC) method [14–16]. However, this method like other simulation techniques is not only laborious and time consuming, but also expensive and not as enlightening as the continuum mechanics approach with regard to the physical insights into the phenomena of interest. Furthermore, it cannot be used if the Knudsen number is less than approximately 0.1 and the mean molecular spacing is much larger than the molecular diameter; see Ref. [15] for a discussion on this aspect. Nevertheless, the DSMC method has been serving as a valuable theoretical tool of investigation in the region of fluid dynamic conditions not met by the NSF equations.

The generalized hydrodynamic equations [17–21] were developed some years ago as a set of macroscopic evolution equations attendant to a theory of irreversible processes in matter. Being an integral part of such a thermodynamic theory of irreversible processes [22], the generalized hydrodynamic equations are manifestly consistent with the laws of thermodynamics. Therefore we now are presented with a tantalizing prospect of studying in a thermodynamically consistent manner and in good accuracy various nonlinear flow phenomena that were beyond the capability of description by the classical hydrodynamic equations, namely, the Navier-Stokes-Fourier equations. As an example of applications for the generalized hydrodynamic equations to nonlinear flow phenomena occurring in fluids far removed from equilibrium, we have recently studied [23] shock wave phenomena in monatomic gases in the case of one-dimensional flow configuration. The shock solutions not only have been found to exist for all Mach numbers, but also the numerical results for the shock structures have been found excellent in comparison with experimental data available in the literature. We thus have demonstrated that there are continuum mechanical equations for hydrodynamic field variables in the forms of generalized hydrodynamic equations that are capable of describing shock phenomena as well as other flow phenomena with sufficient numerical precision. The theory is relatively easy to implement numerically with a fraction of cost and labor compared with the DSMC method. The theory has been implemented for two- or three-dimensional shock waves by Myong [24,25] with excellent numerical results for all Mach numbers studied. Myong and his collaborators [26,27] also have successfully applied the theory to gas dynamics problems, showing that it can treat the aspects of flow that cannot be handled by the Navier-Stokes theory and

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yields results comparable with the DSMC method. Therefore, it is fair to say that we are now in possession of a continuum mechanical theory capable of describing flow phenomena in monatomic fluids in the forms of generalized hydrodynamic equations. These equations are not only inclusive of the classical Navier-Stokes-Fourier theory in the low Mach number regime but also thermodynamically consistent for all Mach numbers.

To study flow phenomena in molecular fluids the aforementioned generalized hydrodynamic equations for monatomic gases must be suitably extended to such fluids. In a recent work [28] on ultrasonic wave absorption and dispersion in diatomic gases such as nitrogen, hydrogen, deuterium, and deuterium hydride, thermodynamically consistent generalized hydrodynamic equations for molecular fluids have been derived from the Boltzmann-Curtiss equation [29] for rigid molecules and applied to study ultrasonic wave absorption and dispersion coefficients as functions of frequency and temperature. To implement the theory for sound wave phenomena a linearization of the equations was necessarily required so that the usual Fourier transform method could be applied. Although such a linearization of the equations tends to reduce the numerical accuracy, the good results obtained for the ultrasonic absorption and dispersion coefficients that agree with experiment over a sufficiently wide range of frequency were rather encouraging and indicative of the utility of the generalized hydrodynamic equations for other flow problems of the molecular gases studied.

In this work, by gleaning the generalized hydrodynamic equations derived from the Boltzmann-Curtiss kinetic equation and used for the aforementioned study of ultrasonic absorption and dispersion and by suitably fashioning them on the phenomenological grounds in a manner consistent with the laws of thermodynamics, we formulate a set of continuum mechanical (hydrodynamic) equations that can be reliably used for flow problems of molecular fluids. In this paper we specifically propose such a set of generalized hydrodynamic equations for flow problems for molecular gases on the phenomenological grounds and, by applying them to study shock waves in nitrogen gas, investigate their utility in comparison of the theoretical results with experimental data. Therefore *our approach is phenomenological and deductive*; there is no kinetic theory involved in the present theory; and the proposition made for the evolution equations for macroscopic variables is justified *a posteriori* in comparison with experiment. The capability of a shock wave theory can be succinctly symbolized by the Mach number dependence of shock width, which may be regarded as the touchstone for the veracity of a shock wave theory. In shock wave theory it is not sufficient to calculate and show shock profiles for only a few cases of Mach number. We will show that the inverse shock widths [30] of nitrogen computed are in excellent agreement with experiment up to Mach number 10 reported in the literature [31–35]. The potential range of utility of the theory, however, extends well beyond the range of Mach number numerically investigated in this work, as suggested by the analysis made of the singularities of the direction field of the evolution equations for velocity and temperature.

In Sec. II the generalized hydrodynamic equations for diatomic fluids are presented in general form. They are then specialized to the case of one-dimensional shock waves. The one-dimensional equations are then reduced by using suitable reference variables in Sec. III. The one-dimensional shock waves can be described by two variables, velocity and temperature. The evolution equations for velocity and temperature are presented in this section, where the boundary conditions are also discussed together with direction fields and singularities of the direction field equation. From the consideration of the nature of the singularities and the direction field it is possible to conclude that the shock solutions should exist for all Mach numbers in the case of one-dimensional generalized hydrodynamic equations formulated. The numerical results obtained from the aforementioned evolution equations for velocity and temperature are used to calculate shock profiles for various field variables and, most importantly, the inverse shock widths in Sec. IV. The latter results are in excellent agreement with the experimental data available in the literature. Section V is for discussion and concluding remarks.

II. GENERALIZED HYDRODYNAMIC EVOLUTION EQUATIONS

A. Generalized hydrodynamic equations for three dimensions

In the case of molecular fluids the hydrodynamic field variables necessary for an appropriate description of flow in the fluids may consist of density ρ, velocity $\mathbf{u}$, internal energy $\mathcal{E}$, heat flux $\mathbf{Q}$, and stress tensor $\mathbf{P}$, which may be decomposed into the shear stress $\mathbf{\Pi}$, the excess normal stress Δ, and pressure p, in addition to the energy for the internal degrees of freedom and rotational angular momentum. The internal degrees of freedom evolve on a faster time scale than the other hydrodynamic variables mentioned, unless their relaxation is inhibited for the reason of low temperature or other causes. We will assume that their relaxation is faster than the hydrodynamic variables. This implies that the evolution equations for the internal degrees of freedom may be suppressed in the present theory. Therefore in addition to the usual conservation laws of mass, momentum, and the internal energy, there are the constitutive equations for the heat flux and the stress tensor—nonconserved variables—to describe shock phenomena in the diatomic gas of interest. For the sake of generality we first present them in general form [20,21]:

$$\rho \frac{dv}{dt} = \nabla \cdot \mathbf{u} \quad (v = 1/\rho), \tag{1}$$

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla \cdot (\mathbf{\Pi} + \Delta \boldsymbol{\delta} + p \boldsymbol{\delta}), \tag{2}$$

$$\rho \frac{d\mathcal{E}}{dt} = -\nabla \cdot \mathbf{Q} - (\mathbf{\Pi} + \Delta \boldsymbol{\delta} + p \boldsymbol{\delta}) : \nabla \mathbf{u}, \tag{3}$$

where $d/dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the substantial time derivative and $\boldsymbol{\delta}$ is the unit second rank tensor. In these equations the stress tensor $\mathbf{P}$ is decomposed into three parts

$$\mathbf{P}=\mathbf{\Pi}+\Delta\boldsymbol{\delta}+p\boldsymbol{\delta}, \tag{4}$$

where $\mathbf{\Pi}$ and Δ are, respectively, the traceless symmetric part and the excess normal stress part of $\mathbf{P}$ and p is the hydrostatic pressure. The excess normal stress part has to do with the bulk viscosity of the fluid, which does not exist in the case of dilute monatomic gases. The pressure is described by a suitable equation of state, which in the case of dilute gases is the ideal gas equation of state. The nonconserved variables $\mathbf{\Pi}$, Δ, and $\mathbf{Q}$ are described by their evolution equations that we propose to have the forms [28]

$$\rho\frac{d\hat{\mathbf{\Pi}}}{dt}=-2(p+\Delta)[\boldsymbol{\nabla}\mathbf{u}]^{(2)}-2[\mathbf{\Pi}\cdot\boldsymbol{\nabla}\mathbf{u}]^{(2)}-\frac{p}{\eta_0}\mathbf{\Pi}q(\kappa), \tag{5}$$

$$\rho\frac{d\hat{\mathbf{Q}}}{dt}=-(p+\Delta)\hat{C}_pT\boldsymbol{\nabla}\ln T-\mathbf{\Pi}\cdot\boldsymbol{\nabla}\hat{h}-\mathbf{Q}\cdot\boldsymbol{\nabla}\mathbf{u}+\boldsymbol{\nabla}\cdot(p\boldsymbol{\delta}+\Delta\boldsymbol{\delta}+\mathbf{\Pi})\cdot(\hat{\mathbf{\Pi}}+\hat{\Delta}\boldsymbol{\delta})-\frac{p\hat{C}_pT}{\lambda_0}\mathbf{Q}q(\kappa), \tag{6}$$

$$\rho\frac{d\hat{\Delta}}{dt}=-\frac{2}{3}\frac{\hat{C}_v^{(r)}}{\hat{C}_v}(\Delta\boldsymbol{\delta}+\mathbf{\Pi}):\boldsymbol{\nabla}\mathbf{u}-\frac{2}{3}\frac{\hat{C}_v^{(r)}}{\hat{C}_v}p\boldsymbol{\nabla}\cdot\mathbf{u}-\frac{2}{3}\frac{\hat{C}_v^{(r)}}{\hat{C}_v}\frac{p}{\eta_b}\Delta q(\kappa). \tag{7}$$

The set of field equations for the variables $(\rho,\mathbf{u},\mathcal{E},\mathbf{\Pi},\mathbf{Q},\Delta)$ presented above constitutes the generalized hydrodynamic equations for flows in rigid diatomic gases. The symbol $[\mathbf{A}]^{(2)}$ stands for the traceless symmetric part of tensor $\mathbf{A}$. For example, in the case of the velocity gradient $\boldsymbol{\nabla}\mathbf{u}$ it means $[\boldsymbol{\nabla}\mathbf{u}]^{(2)}=[\boldsymbol{\nabla}\mathbf{u}+(\boldsymbol{\nabla}\mathbf{u})^t]/2-\boldsymbol{\delta}\boldsymbol{\nabla}\cdot\mathbf{u}/3$. Other symbols are as follows: $\hat{\mathbf{\Pi}}=\mathbf{\Pi}/\rho$; $\hat{\Delta}=\Delta/\rho$; $\hat{\mathbf{Q}}=\mathbf{Q}/\rho$; $\hat{C}_p$ and $\hat{C}_v$ are the specific heat per mass at constant pressure and at constant volume, respectively; $\hat{C}_v^{(r)}$ is the rotational specific heat per mass of the molecule; $\hat{h}=\hat{C}_pT$ is the enthalpy per mass; η_0, η_b, and λ_0 are the shear viscosity, bulk viscosity, and thermal conductivity (more precisely, the Fourier thermal conductivity times T) [36] of the molecular gas, respectively; and finally $q(\kappa)$ is a nonlinear factor [17,20,21] defined by

$$q(\kappa)=\frac{\sinh\kappa}{\kappa}, \tag{8}$$

where κ^2 is the Rayleigh dissipation function for the process in question

$$\kappa=\frac{(mk_BT)^{1/4}}{\sqrt{2}pd}\left(\frac{1}{2\eta_0}\mathbf{\Pi}:\mathbf{\Pi}+\frac{C_v^{(r)}}{C_v}\frac{1}{\eta_b}\Delta^2+\frac{1}{\lambda_0}\mathbf{Q}\cdot\mathbf{Q}\right)^{1/2}. \tag{9}$$

Here d denotes the size parameter of the molecule and m is the molecular mass. In fact, d may be taken as the mean diameter of the molecule in the case of a diatomic molecule. It may be identified with the size parameter in the potential energy model for the diatomic gas in practice. The $q(\kappa)$ is the factor much responsible for the nonlinear behavior of the material functions for the gas and also for the nonlinear modes of energy dissipation in the gas. The calortropy production is a local representation of the second law of thermodynamics and the system of evolution equations presented is consistent with the second law of thermodynamics in the sense that the calortropy production given by

$$\Xi=k_B\kappa\sinh\kappa\geqslant 0 \tag{10}$$

is positive for all values of the nonconserved variables. In the sense that the first and second law of thermodynamics are satisfied by the generalized hydrodynamic equations presented, the latter are therefore thermodynamically consistent, and so is the theory of shock waves developed here for diatomic fluids.

Although Eqs. (5)–(7) together with the Rayleigh dissipation function κ^2 are assumed as phenomenological equations, they can be shown to have some kinetic theory basis if the Boltzmann-Curtiss equation for rigid diatomic gases [29] or a suitable kinetic equation for diatomic gases [37,38] is used and if the closure is chosen such that the macroscopic variables are limited to only those elements in the set $(\rho,\mathbf{u},\mathcal{E},\mathbf{\Pi},\mathbf{Q},\mathbf{\Delta})$. For the kinetic theory justification and examination of the approximations necessary to obtain the evolution equations postulated in this work, see Ref. [28] where the method of obtaining the evolution equations for macroscopic variables are given within the framework of the nonequilibrium ensemble method [20,21]. However, in the reference just quoted, only linearized versions of the constitutive equations are presented and used. We have shown in a number of studies [20,39–44] on nonlinear transport coefficients that the constitutive equations (5) and (6) give rise to sufficiently accurate nonlinear transport coefficients, and particularly non-Newtonian viscosities, in comparison with experiments. The new addition to the generalized hydrodynamic equations, Eq. (7) for Δ, appears in a linearized form in the ultrasonic wave study mentioned [28]; it has to do with the bulk viscosity of the gas. With this new addition, the generalized hydrodynamic equations have yielded rather encouraging results on absorption and dispersion characteristics. On the strength of this finding, we have postulated the evolution equations for the shock wave problem presented. In this work, we are using a deductive approach to the shock wave problem by making a postulate for the continuum hydrodynamic equations and justify their utility *a posteriori* in comparison with experiment.

The equations (5)–(7) generalize the constitutive equations, namely, the evolution equations, for the nonconserved variables in the generalized hydrodynamics previously reported for monatomic fluids [23], because the transport coefficients, the enthalpy density, and specific heats are all for diatomic gases, and furthermore there is the equation for the excess normal stress Δ together with the attendant bulk viscosity. In the event that in the domain of some physical parameters, such as temperature or the frequency of an external force, where the relaxation times of rotational energy

and angular momentum are comparable to the hydrodynamic relaxation times, the rotational energy and angular momentum evolution equations should be added to the set of evolution equations presented earlier. These aspects will be deferred to a later study, when the present approximation is ascertained of its validity.

B. One-dimensional shock wave equations

We assume that flow is in the direction of the x coordinate in a fixed coordinate system and the flow may be approximated as one-dimensional, with the transversal components of the macroscopic variables in the set $(\rho,\mathbf{u},\boldsymbol{\mathcal{E}},\boldsymbol{\Pi},\mathbf{Q},\Delta)$ put equal to zero. This, however, represents an approximation of two- or three-dimensional shock wave phenomena experimentally or naturally observed. Since we are interested in a steady shock wave in the flow configuration assumed, the conservation laws for mass, momentum, and energy are time independent and have the forms

$$\frac{d}{dx}\rho u=0, \tag{11}$$

$$\frac{d}{dx}(\rho u^2+p+\Delta+\Pi_{xx})=0, \tag{12}$$

$$\frac{d}{dx}\left[\rho u\left(\mathcal{E}+\frac{1}{2}u^2\right)+u(p+\Delta+\Pi_{xx})+Q_x\right]=0, \tag{13}$$

where u is the x component of the fluid velocity $\mathbf{u}$, namely, $\mathbf{u}=(u,0,0)$, p is the pressure given by the ideal gas equation of state, Π_{xx} is the xx component of the shear stress, and Q_x is the x component of the heat flux. We note that in the one-dimensional flow configuration assumed for the present problem

$$[\boldsymbol{\nabla}\mathbf{u}]^{(2)}_{xx}=\frac{2}{3}\partial_x u. \tag{14}$$

The balance equations (11)–(13) are supplemented by the evolution equations for Π_{xx} and Q_x.

The nonconserved variables such as $\boldsymbol{\Pi}$ and $\mathbf{Q}$ vary on a faster time scale than the conserved variables such as the density, energy (or temperature), and momentum (or fluid velocity). Therefore, on the time scale of variation in the conserved variables the nonconserved variables have already reached their steady state, and it can be shown, by scaling the substantial time derivative terms in the constitutive equations with the Deborah number $N_{De}=\tau_s/\tau_h$ or the Q number $N_Q=\tau_q/\tau_h$ where τ_s is the characteristic time of stress relaxation, τ_q is the characteristic time for heat flow, and τ_h is the characteristic time of flow, that the following approximate constitutive equations hold for $\boldsymbol{\Pi}$ and $\mathbf{Q}$:

$$-2(p+\Delta)[\boldsymbol{\nabla}\mathbf{u}]^{(2)}-2[\boldsymbol{\Pi}\cdot\boldsymbol{\nabla}\mathbf{u}]^{(2)}-\frac{p}{\eta_0}\boldsymbol{\Pi}q(\kappa)=\mathbf{0}, \tag{15}$$

$$-(p+\Delta)\hat{C}_pT\boldsymbol{\nabla}\ln T-\boldsymbol{\Pi}\cdot\boldsymbol{\nabla}\hat{h}-(\Delta\boldsymbol{\delta}+\boldsymbol{\Pi})\cdot\frac{d\mathbf{u}}{dt}-\mathbf{Q}\cdot\boldsymbol{\nabla}\mathbf{u}-\frac{p\hat{C}_pT}{\lambda_0}\mathbf{Q}q(\kappa)=\mathbf{0}, \tag{16}$$

$$-2\frac{\hat{C}_v^{(r)}}{\hat{C}_v}(\Delta\boldsymbol{\delta}+\boldsymbol{\Pi}):\boldsymbol{\nabla}\mathbf{u}-\frac{2}{3}\frac{\hat{C}_v^{(r)}}{\hat{C}_v}p\boldsymbol{\nabla}\cdot\mathbf{u}-\frac{2}{3}\frac{\hat{C}_v^{(r)}}{\hat{C}_v}\frac{p}{\eta_b}\Delta q(\kappa)=0. \tag{17}$$

This approximation is called the adiabatic approximation. The adiabatic approximation is valid when the nonconserved variables relax at a much faster time scale than the conserved variables. It is discussed in Refs. [20] and [21] to which the reader is referred for details. The aforementioned scaling argument in essence enables us to neglect the substantial time derivative terms in the constitutive equations in the limits of large N_{De} and N_Q. The utility of this adiabatic approximation has been successfully tested for a number of flow problems [21,23]. We use these constitutive equations in the present work on shock waves.

In the case of the aforementioned one-dimensional flow configuration and the assumption on the vanishing transversal components of the macroscopic variables made for the present problem, the steady-state constitutive equations for Π_{xx}, Q_x, and Δ are obtained from Eqs. (15)–(17) as follows:

$$\frac{p}{\eta_0}\Pi_{xx}q(\kappa)+\frac{4}{3}\Pi_{xx}\partial_x u+\frac{4}{3}p\partial_x u+\frac{4}{3}\Delta\partial_x u=0, \tag{18}$$

$$\frac{\hat{h}p}{\lambda_0}Q_xq(\kappa)+Q_x\partial_x u+(\Pi_{xx}+\Delta)u\partial_x u+\hat{h}(p+\Delta+\Pi_{xx})\partial_x\ln T=0, \tag{19}$$

$$\frac{p}{3\eta_b}\Delta q(\kappa)+\left(\Delta+\Pi_{xx}+\frac{1}{3}p\right)\partial_x u=0. \tag{20}$$

Equations (18)–(20) are partial differential equations for velocity component u and temperature T. We emphasize that there do not appear partial derivatives of Π_{xx} and Q_x in these equations because of the adiabatic approximation.

C. Reduced equations for shock waves

Integration of the balance equations (11)–(13) yields

$$\rho u=M, \tag{21}$$

$$\rho u^2+p+\Delta+\Pi_{xx}=P, \tag{22}$$

$$2\rho u\left(\mathcal{E}+\frac{1}{2}u^2\right)+2u(p+\Delta+\Pi_{xx})+2Q_x=Q, \tag{23}$$

where M, P, and Q are integration constants with the dimension of momentum per volume, momentum flux per volume, and energy flow per volume, respectively. These equations

are also supplemented by the equation of state and the caloric equation of state for the diatomic gas

$$p=\rho\mathcal{R}T, \quad \mathcal{E}=\frac{5}{2}\mathcal{R}T, \tag{24}$$

where $\mathcal{R}$ is the gas constant per mass. Because the rigid diatomic gas is dilute, there is no contribution to the equation of state from the internal degrees of freedom.

Let us define dimensionless variables

$$v=uMP^{-1}, \quad \theta=\mathcal{R}TM^2P^{-2}, \quad \phi=pP^{-1}, \quad r=\rho PM^{-2}, \tag{25}$$

$$\sigma=\Pi_{xx}P^{-1}, \quad \varphi=Q_xQ^{-1}, \quad \psi=\Delta P^{-1}, \alpha=MQP^{-2}.$$

The reduced distance is given by $\xi=xl^{-1}$ where the length scale is provided by the mean free path l defined by

$$l=\frac{\eta_{01}}{\rho_1 u_1}. \tag{26}$$

In this expression and henceforth the subscript 1 refers to the upstream, whereas the downstream will be designated by subscript 2; therefore ρ_1 is the upstream density and η_{01} is the upstream Newtonian viscosity at the upstream temperature T_1.

The transport coefficients η_0, η_b, and λ_0 are reduced with respect to the upstream transport coefficients η_{01} and λ_{01}, respectively:

$$\eta^*=\frac{\eta_0}{\eta_{01}}, \quad \eta_b^*=\frac{\eta_b}{\eta_{01}}, \quad \lambda^*=\frac{\lambda_0}{\lambda_{01}}. \tag{27}$$

With the reduced variables defined in Eqs. (25)–(27) we cast Eqs. (21)–(24) in the forms

$$\begin{gathered}\phi=r\theta,\\ rv=1,\\ rv^2+\phi+\sigma+\psi=1,\\ rv^3+7\phi v+2\sigma v+2\psi v+2\alpha\varphi=\alpha.\end{gathered} \tag{28}$$

On reducing constitutive equations (18)–(20) and using Eq. (28) the following six equations can be obtained for six variables ϕ, θ, v, σ, φ, and ψ:

$$\phi v=\theta, \tag{29}$$

$$v+\phi+\sigma+\psi=1, \tag{30}$$

$$v^2+7\theta+2\sigma v+2\psi v+2\alpha\varphi=\alpha, \tag{31}$$

$$\frac{1}{\eta^*}\phi\sigma q(\kappa)+\frac{4}{3}(\sigma+\psi+\phi)\partial_\xi v=0, \tag{32}$$

$$\frac{\alpha\beta}{\lambda^*}\theta\varphi\phi q(\kappa)+(\alpha\varphi+v\sigma+v\psi)\partial_\xi v+\frac{7}{2}\theta(\phi+\sigma+\psi)\partial_\xi\ln\theta=0, \tag{33}$$

$$\frac{1}{\eta_b^*}\phi\psi q(\kappa)+\left(\sigma+\psi+\frac{1}{3}\phi\right)\partial_\xi v=0. \tag{34}$$

Here the new dimensionless parameter β is defined by

$$\beta=\frac{N_{\mathrm{Pr}}}{\theta_1} \tag{35}$$

with θ_1 denoting the reduced upstream temperature, and N_{Pr} the Prandtl number defined with the upstream quantities:

$$N_{\mathrm{Pr}}=\left(\frac{C_p}{C_v}\right)f_E^{-1}. \tag{36}$$

In this formula f_E is the Eucken number [36] defined for a diatomic gas as

$$f_E=\frac{5}{2}\frac{C_{tr}}{C_v}+\frac{C_{rot}}{C_v}. \tag{37}$$

The Eucken number is usually temperature and density dependent. However, we will assume that it is a constant. Therefore, $N_{\mathrm{Pr}}=14/19$ for a rigid diatomic gas.

The Rayleigh dissipation function κ^2 is reduced as follows:

$$\kappa=N_M\pi^{1/4}\sqrt{\frac{\gamma_0}{2}}\frac{\theta^{1/4}}{\phi\sqrt{\eta^*}}\left(\sigma^2+\frac{4}{5}\frac{\eta^*}{\eta_b^*}\psi^2+2\varepsilon\frac{\eta^*}{\lambda^*}\varphi^2\right)^{1/2}, \tag{38}$$

where

$$\varepsilon=\frac{49}{24}\sqrt{\frac{\pi\gamma_0}{2}}N_M\left[1-25\left(\frac{N_M^2-1}{7N_M^2+5}\right)^2\right] \tag{39}$$

and γ_0 is the polytropic ratio defined by $\gamma_0=C_p/C_v$. We note that the upstream Mach number N_M is defined by

$$N_M=\frac{u_1}{\sqrt{\frac{7}{5}\mathcal{R}T_1}}=\frac{u_1}{u_r}, \tag{40}$$

where u_r is the reference speed which is taken to be the sound speed in the upstream. Therefore the parameter α is related to N_M as follows:

$$N_M=\sqrt{\frac{1+\frac{1}{7}\mu}{1-\frac{1}{5}\mu}}, \tag{41}$$

where

$$\mu=\sqrt{49-24\alpha}. \tag{42}$$

The parameter μ ranges from 0 to 5 at which $N_M=\infty$. Therefore $\alpha=1$ at $N_M=\infty$.

D. Boundary conditions

To determine the boundary conditions on v, ϕ, and θ, we observe that $\sigma\to 0$ and $\varphi\to 0$ as $\xi\to\pm\infty$. Equations (32) and (33) are identically satisfied in the limits, if v and θ become independent of ξ at the boundaries. Therefore, as $\xi\to\pm\infty$,

$$\sigma,\varphi,\psi\to 0, \tag{43}$$

$$\theta=\phi v, \tag{44}$$

$$v+\phi=1, \tag{45}$$

$$v^2+7\theta=\alpha. \tag{46}$$

The solutions of Eqs. (44)–(46) are

$$v=\frac{1}{12}(7\pm\mu), \tag{47}$$

$$\phi=\frac{1}{12}(5\mp\mu), \tag{48}$$

$$\theta=\frac{1}{144}(7\pm\mu)(5\mp\mu). \tag{49}$$

The upper sign is for the upstream and the lower sign is for the downstream. These solutions provide the boundary conditions at the upstream and downstream. They also imply that on account of the equation of state the reduced density is given by

$$r=\frac{12}{7\pm\mu}. \tag{50}$$

E. Differential equations for reduced velocity and temperature

With the help of Eqs. (29)–(33), we can calculate the reduced excess normal stress ψ as a function of v and θ only

$$\psi=\frac{\left(1-v-\frac{2\theta}{3v}\right)\left(1-v-\frac{\theta}{v}\right)}{\left[\frac{4}{3}\frac{\eta^*}{\eta_b^*}(1-v)+\left(1-v-\frac{2\theta}{3v}\right)\right]}. \tag{51}$$

On elimination of variables other than v and θ the differential equations (32) and (33) may be cast into the forms

$$\frac{dv}{d\xi}=\frac{3\theta}{4\eta^* v^2(1-v)}(v^2-v+\theta+v\psi)q(\kappa), \tag{52}$$

$$\frac{d\theta}{d\xi}=-\frac{\theta}{7v^2(1-v)^2}\left[\frac{3(\alpha-v^2-7\theta)(v^2-v+\theta)}{4\eta^*}+\frac{\beta\theta v(1-v)(\alpha+v^2-5\theta-2v)}{\lambda^*}+\frac{3(\alpha-v^2-7\theta)v\psi}{4\eta^*}\right]q(\kappa). \tag{53}$$

These evolution equations for reduced velocity and temperature are solved for shock profiles, subject to the boundary conditions in Eqs. (47)–(49). These equations generalize the evolution equations for v and θ in the Navier-Stokes-Fourier theory as will be discussed presently, and also those in the generalized hydrodynamic theory of one-dimensional shock waves for monatomic gases on which we have reported previously [23].

III. SHOCK SOLUTIONS OF THE EVOLUTION EQUATIONS

The second term on the right-hand side of Eq. (53) stems from the thermoviscous effect involving the second and third terms as well as the term $\hat{h}\Pi_{xx}\partial_x \ln T$ in Eq. (19). These, together with the second term in Eq. (18), are the terms that do not appear in the Navier-Stokes-Fourier theory [45] of the classical hydrodynamics. To indicate the difference between the evolution equations in the classical Navier-Stokes-Fourier theory and the present theory and also to facilitate the solution procedure for Eqs. (52) and (53), we present the evolution equations for one-dimensional shock waves in the Navier-Stokes-Fourier theory

$$\frac{dv}{d\xi}=\frac{(v^2-v+\theta)}{\left(\frac{4}{3}\eta^*+\eta_b^*\right)v}, \tag{54}$$

$$\frac{d\theta}{d\xi}=-\frac{\theta\beta(\alpha+v^2-2v-5\theta)}{7\lambda^*}. \tag{55}$$

These equations follow from Eqs. (29)–(34) if $q(\kappa)$ is set equal to unity and if σ, φ, and ψ are set equal to zero in the second term in Eq. (32), in the second and third terms in Eq. (33), and in the second term in Eq. (34) so that Eqs. (32)–(34) become, respectively, the Newtonian law of viscosity, the Fourier law of heat conduction, and the bulk viscosity law. Since the full set of equations (29)–(34) gives rise to Eqs. (52) and (53), clearly Eqs. (54) and (55) are special cases of Eqs. (52) and (53). If the bulk viscosity is set equal to zero, Eqs. (54) and (55) become the evolution equations considered in the Navier-Stokes-Fourier theory for monatomic gases [45].

We note that in the case of a rough hard sphere gas the reduced transport coefficients η^* and λ^* depend on θ only as follows [36]:

$$\eta^*=\left(\frac{\theta}{\theta_1}\right)^{1/2}, \quad \lambda^*=\left(\frac{\theta}{\theta_1}\right)^{3/2}. \tag{56}$$

To facilitate comparison of the present evolution equations with the evolution equations in the literature, we note the relation between the reduced distance ξ in the present work with the reduced distance z in the literature:

$$z=\frac{x}{l_1}, \tag{57}$$

where l_1 is the upstream mean free path defined with the upstream velocity instead of the upstream sound speed. This relation is important to remember when the shock width is calculated and compared with the literature value.

The evolution equations (52) and (53) are quite different from the evolution equations for σ and φ appearing in the moment equation approach of Grad [46]. The evolution equations in the latter approach, which are differential equations for the stress tensor and the heat flux, were found to fail to produce shock solutions for $N_M \geqslant 1.65$. In the following we examine the evolution equations (52) and (53) and the existence of shock solutions with the help of singularities of the direction field equation [47].

Here in order to gain some insights into the evolution equations obtained for shock waves we will examine the evolution equations in the case of the transport coefficients satisfying Eq. (56) for the relative simplicity of the equations. For the Navier-Stokes-Fourier theory the direction field equation is given by

$$\frac{dv}{d\theta}=-\frac{\omega(v^2-v+\theta)}{v(\alpha+v^2-2v-5\theta)}, \tag{58}$$

where

$$\omega=\frac{\left(\frac{4}{3}\eta^*+\eta_b^*\right)\beta\theta}{7\lambda^*}. \tag{59}$$

It is independent of θ for the transport coefficients obeying Eq. (56). The singularities of the direction field are given by

$$(v^2-v+\theta)=0,$$

$$v(v^2-2v-5\theta+\alpha)=0, \tag{60}$$

which give rise to three singular points P_0, P_1, and P_2:

$$P_0: \quad v=\frac{1}{12}(7+\mu), \quad \theta=\frac{1}{144}(35-2\mu-\mu^2),$$

$$P_1: \quad v=\frac{1}{12}(7-\mu), \quad \theta=\frac{1}{144}(35+2\mu-\mu^2), \tag{61}$$

$$P_2: \quad v=0, \quad \theta=0.$$

Note that P_0 and P_1 coincide with the boundary values given in Eqs. (47) and (49). We remark that P_0 and P_1 are also the singular points of the evolution equations (54) and (55) for the NSF theory where the derivatives $dv/d\xi$ and $d\theta/d\xi$ vanish. It can be shown, by calculating the eigenvalues of the linearized governing equations, that P_0 is a saddle point whereas P_1 is an unstable node and P_2 is a spiral. The shock solution is a curve connecting P_0 and P_1 as $\xi\to\infty$ from $\xi=-\infty$. It is possible to show that there exists a unique such solution [45,46] for every value of α since the aforementioned nature of P_0 and P_1 remains invariant for all Mach numbers. Therefore, the NSF theory admits shock solutions for all values of Mach number. The problem of the NSF theory is that it yields too narrow shock widths that incorrectly behave with regard to the Mach number.

We now examine the evolution equations (52) and (53) by using the direction field equation

$$\frac{d\theta}{dv}=-\frac{(\alpha-v^2-7\theta)(v^2-v+\theta+v\psi)+\omega' v(1-v)(\alpha+v^2-5\theta-2v)}{7(1-v)(v^2-v+\theta+v\psi)}, \tag{62}$$

where

$$\omega'=\frac{4\eta^*\beta\theta}{3\lambda^*}. \tag{63}$$

The right-hand side of this equation may be written as

$$\frac{\frac{4}{3}\frac{\eta^*}{\eta_b^*}(\alpha-v^2-7\theta)(v^2-v+\theta)+\omega' v(\alpha+v^2-5\theta-2v)\left[\frac{4}{3}\frac{\eta^*}{\eta_b^*}(1-v)+\left(1-v-\frac{2\theta}{3v}\right)\right]}{\frac{28}{3}\frac{\eta^*}{\eta_b^*}(1-v)(v^2-v+\theta)}.$$

It is interesting to see that the nonlinear factor $q(\kappa)$ does not appear in this equation and thus the singularities of the direction field are not affected by the nonlinear factor. From this point we gain the following insight: since the nature of the direction field singularities is the crucial deciding factor for the existence of shock solutions, the fact that $q(\kappa)$ does not appear on the right-hand side of Eq. (62) suggests that the existence of shock solutions is not determined by the nonlinear manner in which energy dissipation occurs in the shock wave, for the nonlinear factor $q(\kappa)$ is intimately related to how energy is dissipated in the system. This nonlinear factor appears to control the range over which the energy dissipation occurs in the shock wave. The singularities of the direction field are given by the equations

$$(1-v)(v^2-v+\theta)=0, \tag{64}$$

$$\omega' v(1-v)(\alpha+v^2-5\theta-2v)\left[1-v+\frac{3\eta_b^*}{4\eta^*}\left(1-v-\frac{2\theta}{3v}\right)\right] + (\alpha-v^2-7\theta)(v^2-v+\theta)=0. \tag{65}$$

The second equation (65) can be written as a product of two factors as follows:

$$(A\theta+B+\sqrt{B^2+AC})(A\theta+B-\sqrt{B^2+AC})=0, \tag{66}$$

where

$$A=7-\frac{5\eta_b^*}{2\eta^*}\omega'(1-v), \tag{67}$$

$$2B=7v(1-v)+v^2-\alpha+\frac{\eta_b^*}{2\eta^*}\omega'(\alpha+v^2-2v) + 5\omega'\left(1+\frac{3\eta_b^*}{4\eta^*}\right)v(1-v)^2, \tag{68}$$

$$C=v(1-v)(\alpha-v^2)+\omega'\left(1+\frac{3\eta_b^*}{4\eta^*}\right)v(1-v)^2 \times(\alpha+v^2-2v). \tag{69}$$

Therefore, Eqs. (64) and (66) indicate that the loci of the infinite and zero slopes of the direction field are either parabolas or ellipses (or closed curves) in the (θ,v) plane. See Fig. 1 where P_0 and P_1 are indicated together with other singularities $P_2, \ldots, P_4$.

The solutions of Eqs. (64) and (65) are obtained as follows. If

$$1-v=0 \tag{70}$$

then

$$(\alpha-1-7\theta)\theta=0, \tag{71}$$

which means

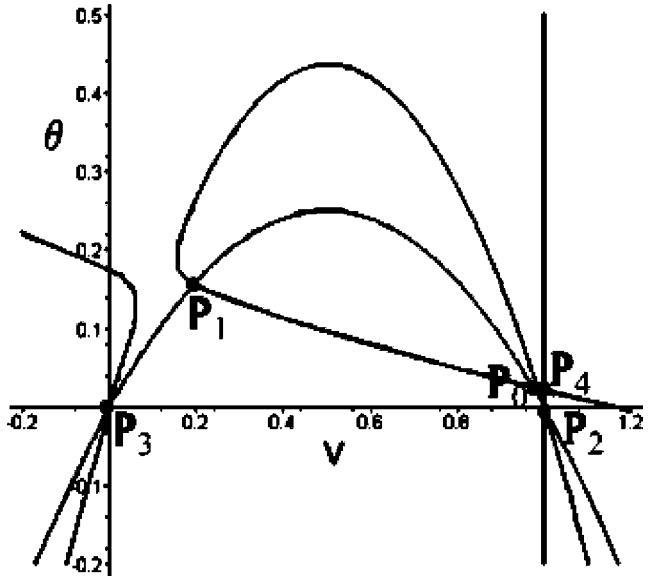

FIG. 1. Loci of zero and infinite slopes in the direction field of the evolution equations for reduced velocity and temperature in the case of $N_M=5$. The intersections of the curves are P_0, P_1, P_2, P_3, and P_4. The shock solutions pass through the bounded region between P_0 and P_1. It can be readily verified that as $N_M\to\infty$, P_1 tends to $P_1(v=1,\theta=0)$. This means that the shock solutions exist for all Mach numbers.

$$\theta=0, \quad \theta=\frac{1}{7}(\alpha-1). \tag{72}$$

If

$$v^2-v+\theta=0, \tag{73}$$

then

$$v(1-v)(\alpha+v^2-5\theta-2v)\left[1-v+\frac{3\eta_b^*}{4\eta^*}\left(1-v-\frac{2\theta}{3v}\right)\right]=0. \tag{74}$$

This means

$$v=0, \quad \theta=0 \tag{75}$$

or

$$(\alpha+v^2-5\theta-2v)=0 \tag{76}$$

or

$$1-v+\frac{3\eta_b^*}{4\eta^*}\left(1-v-\frac{2\theta}{3v}\right)=0. \tag{77}$$

Solving Eqs. (73) and (76), we find

$$v=\frac{7\pm\sqrt{49-24\alpha}}{12},\quad \theta=v-v^2. \tag{78}$$

The other pair is Eqs. (73) and (77) from which follows the equation

$$(1-v)+\frac{\eta_b^*}{4\eta^*}(1-v)=0.$$

This equation is redundant, since it yields the solution that was obtained earlier,

$$v=1,\quad \theta=0.$$

Equations (64) and (65) therefore yield the five singular points $P_0,\ldots,P_4$ given below:

$$\begin{aligned}
P_0:&\quad v=\frac{1}{12}(7+\mu),\quad \theta=\frac{1}{144}(35-2\mu-\mu^2),\\
P_1:&\quad v=\frac{1}{12}(7-\mu),\quad \theta=\frac{1}{144}(35+2\mu-\mu^2),\\
P_2:&\quad v=1,\quad \theta=0,\\
P_3:&\quad v=0,\quad \theta=0,\\
P_4:&\quad v=1,\quad \theta=\frac{1}{7}(\alpha-1)=\frac{1}{168}(25-\mu^2).
\end{aligned} \tag{79}$$

It is useful to compare these singular points with those of the shock wave evolution equation in the case of a vanishing bulk viscosity:

$$\begin{aligned}
P_0:&\quad v=\frac{1}{8}(5+\mu),\quad \theta=\frac{1}{64}(15-2\mu-\mu^2),\\
P_1:&\quad v=\frac{1}{8}(5-\mu),\quad \theta=\frac{1}{64}(15+2\mu-\mu^2),\\
P_2:&\quad v=1,\quad \theta=0,\\
P_3:&\quad v=0,\quad \theta=0,\\
P_4:&\quad v=1,\quad \theta=\frac{1}{5}(\alpha-1)=\frac{1}{80}(9-\mu^2).
\end{aligned} \tag{80}$$

The number of singularities and their structures and natures are similar between the two cases, and the similarity indicates that the present case will also admit shock solutions. The linear analysis of Eq. (62) reveals that P_0 is a saddle and P_1 is an unstable node for all Mach numbers. A shock solution exists whenever one of the singular points is a saddle and the other is an unstable node for a given Mach number. In this case, any trajectory that enters the saddle will slide toward the node, being confined between the curves between P_1 and P_0, and eventually pass through the node out of the confined region between P_1 and P_0. The situation is very similar to a heteroclinic connection in the theory of nonlinear differential equations [48]. In fact, since $\mu\to 5$ as $N_M\to\infty$, it follows that $P_0,P_4\to P_2$, whereas P_1 tends to a point other than P_3. It is significant that P_0 tends toward $P_2=(v=1,\theta=0)$ as $N_M\to\infty$, because this means that the shock solution exists for all Mach numbers. Therefore, the one-dimensional generalized hydrodynamic equations presented describe shock phenomena in one dimension for all Mach numbers, and there remains only the verification of the numerical accuracy of the shock solutions obtained from the differential equations (52) and (53). It must be remembered that the existence of shock solutions does not guarantee the accuracy of the solutions. The verification is done in the following section.

IV. NUMERICAL SOLUTIONS AND COMPARISON WITH EXPERIMENT

Although stiff, the differential equations (52) and (53) are ordinary and straightforward to solve numerically by using a suitable integrator. They are integrated by starting with the boundary conditions specified by Eqs. (47)–(50) at various Mach numbers. The solutions are obtained by using the temperature dependence of reduced transport coefficients in the following forms:

$$\eta^*=\left(\frac{\theta}{\theta_1}\right)^{0.78},\quad \lambda^*=\left(\frac{\theta}{\theta_1}\right)^{1.78},\quad \eta_b^*=\frac{2}{3}\eta^*. \tag{81}$$

These are patterned after the Sutherland model [49] used for monatomic gases interacting through a nonhard sphere potential such as the Lennard-Jones potential. These representations of the temperature dependence of the transport coefficients, generally used in the literature in connection with shock structures, should be taken as empirical relations. The inverse shock width is defined by the usual formula used in shock wave studies

$$\delta=\frac{n_2-n_1}{(dn/dz)_{\max}}, \tag{82}$$

where n_i $(i=1,2)$ denote the number densities and the density derivative is evaluated at the maximum. The transition point $z=0$ or $\xi=0$ is defined by the inflection point of the profile in this work. It is convenient to define the normalized reduced density, velocity, and temperature by the formulas

$$r_n=\frac{r-r_1}{r_2-r_1},\quad v_n=\frac{v-v_2}{v_1-v_2},\quad \theta_n=\frac{\theta-\theta_1}{\theta_2-\theta_1}. \tag{83}$$

In Figs. 2–4 the normalized reduced density, velocity, and temperature profiles are plotted against the reduced distance ξ. The various shock profiles are as follows: dotted curve for $N_M=10$; the dash-dotted curve for $N_M=5$; the broken curve for $N_M=2$; and the solid curve for $N_M=1.2$. The same meanings apply to all shock profiles in this work. In Figs. 5–7 the shock profiles for the reduced stress tensor, heat flux, and excess normal stress are plotted against ξ. These figures show that the nonconserved variables are confined to a narrow region around the transition point $(\xi=0)$ where energy dissipates, causing the velocity rapidly diminished to

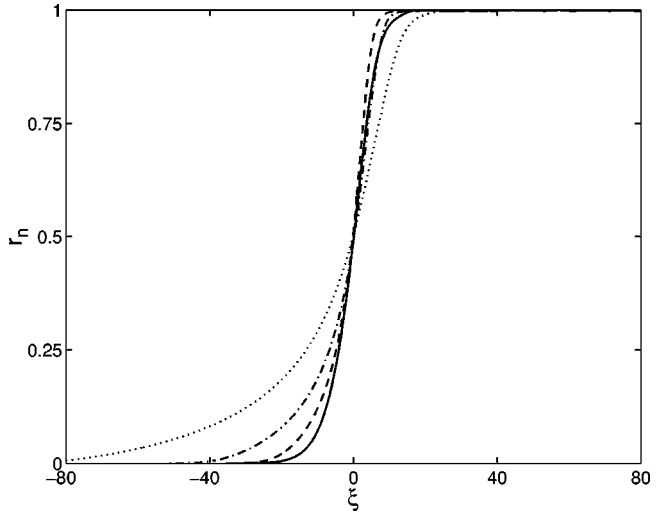

FIG. 2. Normalized reduced density r_n profiles at various Mach numbers. $N_M=1.2$ for the solid curve $(-)$; $N_M=2$ for the broken curve $(--)$; $N_M=5$ for the dash-dotted curve $(-\cdot-)$; $N_M=10$ for the dotted curve $(\cdots)$.

the downstream value. A measure of shock structure is given by the inverse shock width, which is plotted as a function of N_M in Fig. 8, where the filled circles (●) are the values predicted by the present theory and other symbols are experimental values reported in the literature: (▽) by Greene and Hornig [31]; (△) by Linzer and Hornig [32]; (□) by Camac [33]; (×) by Robben and Talbot [34]; and (○) by Alsmyer [35]. The filled circles (theoretical values) are connected by the solid curve to guide the eyes. The broken curve is connecting the inverse shock widths calculated by the Navier-Stokes-Fourier theory. Beyond $N_M\approx 1.6$ the NSF theory gives the inverse shock widths much too large compared with experimental values. The theoretical values are computed up to $N_M=10$, which is the maximum Mach number experimentally studied. As shown in the previous section,

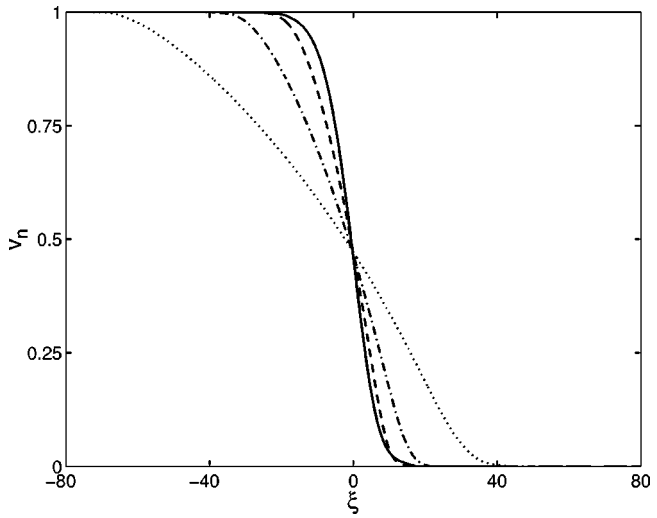

FIG. 3. Normalized reduced velocity v_n profiles at various Mach numbers. The meanings of the curves are the same as in Fig. 2.

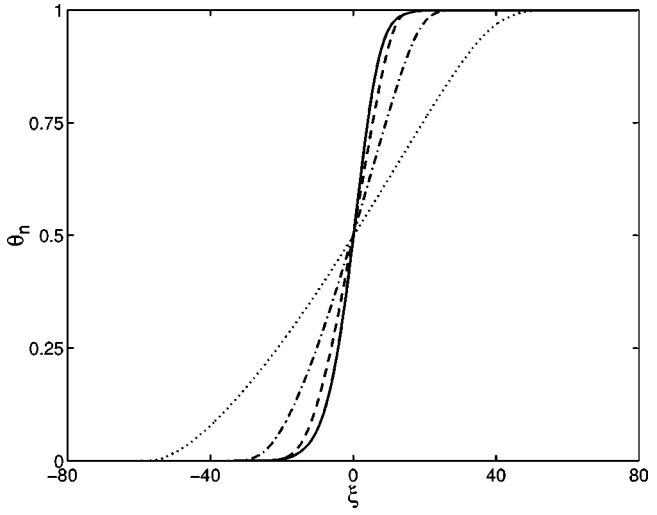

FIG. 4. Normalized reduced temperature (θ_n) profiles at various Mach numbers. The meanings of the curves are the same as in Fig. 2.

the present theory is capable of giving shock solutions for all Mach numbers. The agreement between the theory and experiment is found to be excellent for the entire range of Mach numbers examined experimentally. The comparison presented strongly supports the validity and thus the utility of the phenomenological model based on the generalized hydrodynamics for diatomic fluids. In Fig. 9 the reduced calortropy production Ξ/k_B

$$\Xi/k_B=\kappa\sinh\kappa\geqslant 0, \tag{84}$$

is plotted against N_M. The ordinate EP stands for the reduced calortropy production, which is evidently positive throughout the range examined, suggesting that the second law of thermodynamics is satisfied in the range studied. This calortropy production is a measure of energy dissipation from the useful form (a higher velocity) to a less useful form

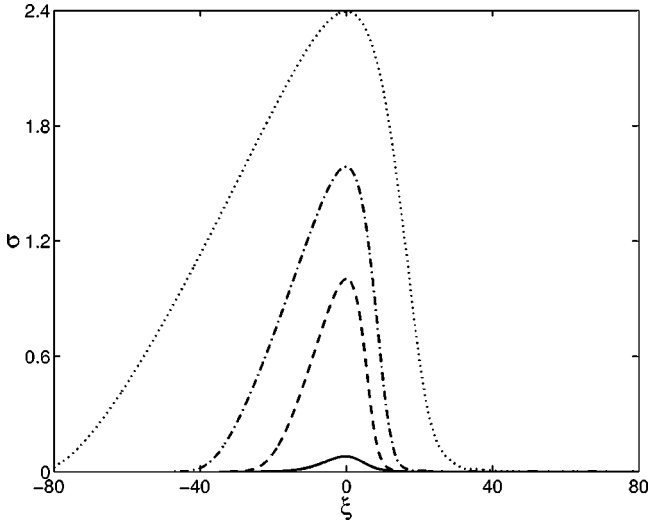

FIG. 5. Reduced stress tensor profiles at various Mach numbers. The meanings of the curves are the same as in Fig. 2.

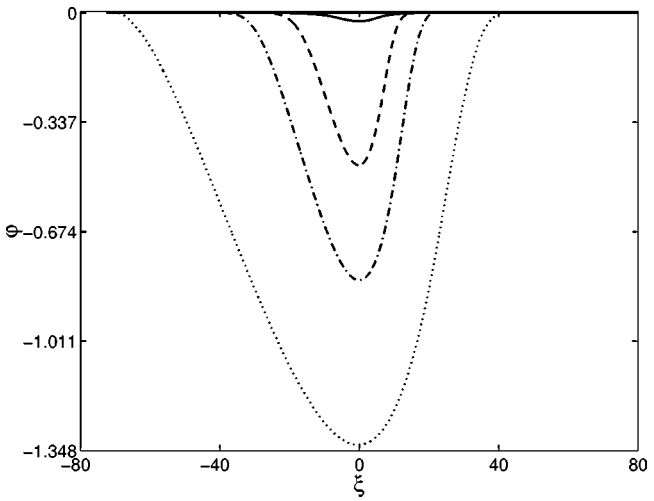

FIG. 6. Reduced heat flux profiles at various Mach numbers. The meanings of the curves are the same as in Fig. 2.

(a lower velocity). Clearly, such energy dissipation occurs in a narrow region around the transition point.

V. DISCUSSION AND CONCLUDING REMARKS

In this paper we have presented a set of phenomenological continuum hydrodynamic equations for shock waves in diatomic gases within the framework of generalized hydrodynamics. The evolution equations are a generalization of the generalized hydrodynamic equations for monatomic fluids, which have been successfully applied to calculate shock wave structures in monatomic gases in our previous paper [23]. As is shown in the preceding section, the theory is successful in accounting for shock wave structures of nitrogen gas. It is emphasized that nitrogen is treated as a rigid rotator in this work unlike in some works in the literature where it is treated as if it is a spherical molecule. As an indicator of the robustness of the theory, the inverse shock widths [30] are calculated over a wide range of Mach number ($1 \leqslant N_M \leqslant 10$). The values of the inverse shock width predicted by the theory are generally in excellent agreement with those measured by a number of authors over a period of many years in the range of N_M experimentally studied.

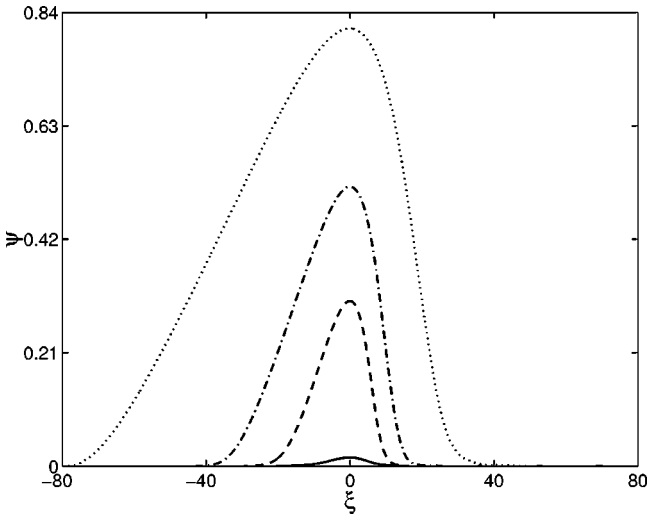

FIG. 7. Reduced excess normal stress profiles at various Mach numbers. The meanings of the curves are the same as in Fig. 2.

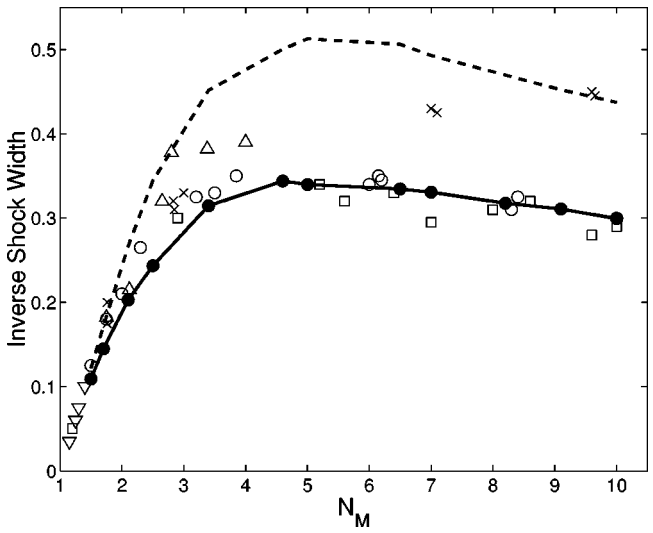

FIG. 8. Inverse shock width vs Mach number. The symbols are: (▽) by Greene and Hornig [31]; (△) by Linzer and Hornig [32]; (□) by Camac [33]; (×) by Robben and Talbot [34]; and (○) by Alsmyer [35]. The filled circles (●) are the values by the present theory and the solid curve connects the theoretical values to guide the eyes. The broken curve is connecting the inverse shock width values calculated by the Navier-Stokes-Fourier theory. The present theory is capable of giving the shock solutions beyond $N_M = 10$ and, in fact, for all Mach numbers.

The generalized hydrodynamic equations presented for shock wave phenomena in diatomic gases have been gleaned from the evolution equations derived in the study [28] made by one of us with his collaborator to calculate ultrasonic wave dispersion and absorption in diatomic gases. And the so constructed generalized hydrodynamic equations are pro-

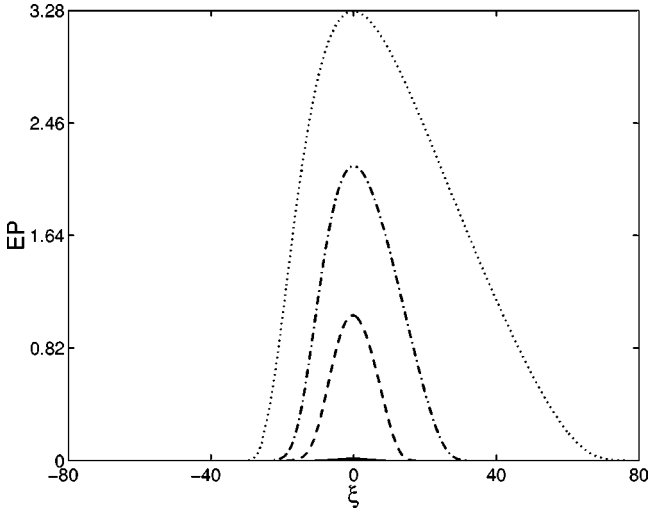

FIG. 9. Reduced calortropy production vs Mach number. The meanings of the curves are the same as in Fig. 2. The ordinate is the reduced calortropy production.

posed as a phenomenological model for shock waves of diatomic gases. They may be generally used for various flow problems of diatomic fluids. The original derivation of the equations was made on the basis of the Boltzmann-Curtiss kinetic equation in order to formulate the theory of irreversible processes in diatomic gases, which is consistent with the laws of thermodynamics. The generalized hydrodynamic equations employed in the present study are thermodynamically consistent in the sense that $\Xi \geqslant 0$ for all values of the nonconserved variables chosen for the description of the flow problem in hand. The requirement of thermodynamic consistency for a theory of macroscopic irreversible processes in matter has important consequences for the theory to accurately account for macroscopic observables. The dissipation terms in the evolution equations for the nonconserved variables such as $\mathbf{\Pi}$, $\mathbf{Q}$, and Δ, which are proportional to $\mathbf{\Pi}q(\kappa)$, $\mathbf{Q}q(\kappa)$, and $\Delta q(\kappa)$ and give rise to the positive calortropy production Ξ defined in Eq. (10) and representing the second law of thermodynamics, play a crucial role in properly describing the important energy dissipation mechanism and thereby enhancing the precision of the theory. The basis for this statement is that if the nonlinear factor $q(\kappa)$ is set equal to unity in the limit of low κ because the nonconserved variables $\mathbf{\Pi}$, $\mathbf{Q}$, and Δ are small in magnitude owing to the fact that the fluid is near equilibrium, then in the adiabatic approximation and on linearization of the resulting equations we recover from the generalized hydrodynamic equations the classical hydrodynamic theory, which predicts unacceptably poor shock structures beyond $N_M \approx 1.6$. Therefore, in the case of diatomic gases, in addition to the contribution from the excess normal stress Δ it is important to have the nonlinear factor $q(\kappa)$ as well as nonlinear kinematic terms—as in Eqs. (15)–(17)—as is for the case of monatomic gases, if we would like to maintain the desired accuracy. The argument κ in the nonlinear factor $q(\kappa)$ is basically the square root of the Rayleigh dissipation function, which gives a measure of energy dissipation in the system. In the general scaling scheme this κ can be scaled by a composite fluid dynamic number [20,21] N_δ proportional to $N_M N_{Kn}$, where N_{Kn} is the Knudsen number. In the shock wave problems the Knudsen number does not explicitly appear when κ is expressed in reduced variables defined earlier in the main text; recall Eq. (38) in which only the Mach number N_M appears. The point we would like to emphasize here is that the reduction scheme for κ should carefully take into consideration the flow problem in hand.

In the present theory of shock waves we have not explicitly taken into account the rotational energy and rotational angular momentum relaxation mechanisms on the basis that in the thermodynamic conditions examined experimentally the aforementioned degrees of freedom relax much faster than the other hydrodynamic modes. These internal degrees of freedom, however, indirectly contribute to the appearance of bulk viscosity in the theory. Therefore, it would be misleading to think that they are ignored completely. If the temperature is sufficiently low or there is a mechanism that retards sufficiently fast relaxations of such internal degrees of freedom, then their evolution equations should be explicitly taken into account in the theory. Investigation of the effects of such evolution equations on flow problems is left for future study. There is no theory that does not need improvement, and there are many aspects we would like to further examine in the present theory, but on the basis of the numerical results presented in this work it is reasonable to tentatively conclude that the generalized hydrodynamic equations presented enable us to study shock wave structures in good accuracy and thus we now have a phenomenological continuum theory of shock wave phenomena on which to build a more complete theory of shock waves of diatomic gases and, perhaps, of more complicated molecules in the future.

Grad's 13-moment method [46] does not yield shock solutions for $N_M \geqslant 1.65$, and the presence of such a maximum Mach number is clearly elucidated by the theorem of Ruggeri [50], who examined the system of moment evolution equations in a general context to establish his theorem. Ruggeri's system of moment evolution equations appears to require a Grad-like closure in which the neglected higher order moments are expressed in terms of the lower order moments retained for the description of the flow problem. Therefore his system is a general form of the Grad's 13-moment evolution equations. Ruggeri's theorem clearly shows that $N_M = 1.65$ is the maximum Mach number beyond which the shock solutions do not exist, given the system of moment evolution equations in the Grad-like closure, and that it is useless to add more and more moments in an attempt to increase the critical Mach number.

The generalized hydrodynamic equations postulated in the present work do not contradict Ruggeri's theorem, because they are not the same system of evolution equations as Ruggeri's system of evolution equations owing to the fact that first the fluxes of the nonconserved variables (e.g., the flux of the stress tensor, the flux of the heat flux, etc.) do not appear in the generalized hydrodynamic equations used and second the spatial derivatives of the nonconserved variables (e.g., the stress tensor and the heat flux) do not appear in the generalized hydrodynamic equations in the adiabatic approximation. These two features combine to produce a system of ordinary differential equations that are quite different from the system of evolution equations considered by Ruggeri, namely, the moment evolution equations in the Grad-like closure. The present generalized hydrodynamic equations consequently do not have a critical Mach number beyond which there are no shock solutions.

We would like to close this section with some remarks on the Burnett equation approach that has been taken by a number of authors in the literature [4–11]. Since these studies are made for monatomic gases, their relevance to the present work is somewhat remote, but we believe it worthwhile to make a remark. Since the Chapman-Enskog expansion is not known to be convergent, the Burnett order constitutive equations used for the stress tensor and heat flux in the aforementioned references should be regarded as an empirical model, just as the present generalized hydrodynamic equations are. Consequently, their thermodynamic consistency must be checked appropriately; it is questionable that they are thermodynamically consistent according to the investigation made in Ref. [21]. Such empirical constitutive equations, nevertheless, appear to improve the Mach number depen-

dence of the inverse shock width in comparison with the classical hydrodynamic theory, but still has a way to go to agree with experimental values within an acceptable accuracy. It is not clear, and is yet to be seen, whether the Burnett order solution for the Boltzmann-Curtiss kinetic equation will provide a similar improvement in the case of molecular gases. To implement a theory in such a direction, first of all, it is necessary to obtain the Burnett order solution for the Boltzmann-Curtiss equation, but it is not available at this point. In any case, we believe that the generalized hydrodynamic equations presented in this work appear to have already met the need for a continuum mechanical (hydrodynamic) theory, albeit from a different standpoint.

ACKNOWLEDGMENTS

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