PHYSICAL REVIEW E VOLUME 52, NUMBER 6 DECEMBER 1995

Continuous shock structure in extended thermodynamics

W. Weiss
Institut für Thermodynamik und Reaktionstechnik, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin
(Received 10 July 1995)

It is shown by numerical calculations that in extended thermodynamics of 13, 14, 20, and 21 moments a continuous shock structure exists up to a critical Mach number. The critical Mach number increases by increasing the number of moments; the value runs from 1.65 for 13 moments up to 1.887 for 21 moments.

PACS number(s): 47.40.Nm, 05.70.Ln

I. INTRODUCTION

The shock structure in monatomic gases is not satisfactorily described by the Navier-Stokes-Fourier theory, e.g., see [1]. But Grad's 13-moment theory is even worse; indeed, Grad [2,3] himself found that no continuous shock structure exists beyond Mach 1.65, which is the maximum speed of propagation of the 13-moment theory. Several methods exist to increase this Mach number [4,5].

We have always thought that the proper manner to improve on the calculation of the shock structure should proceed by taking more and more moments into account. Extended thermodynamics provides hyperbolic systems at every stage—so that there is always a maximum speed of propagation—but that speed increases with the number of moments. Thus the proposition is that with more and more moments the shock structure may be improved up to higher and higher Mach numbers.

This proposition became doubtful when Ruggeri [6] argued that each characteristic speed of the hyperbolic system—not only the maximum speed—produces a singularity. By this argument the higher moment theories should permit a smooth shock structure only for Mach numbers slightly above $M=1$. Therefore, Ruggeri's argument posed a dilemma; it cast doubt on the kinetic theory, and in particular, on the method of moments for calculation of shocks. This situation has motivated our study and in the present paper we remove this doubt. It is true that the shock structure becomes singular at every characteristic speed; but our numerical calculations with 14, 20, and 21 moments show that these singularities are regular, so that the shock structure is smooth until, of course, we reach the maximum speed. Between 13 and 21 moments that maximum speed rises from $M=1.65$ to $M=1.887$.

In a forthcoming paper higher-moment theories will be investigated in the attempt to obtain quantitatively correct shock structures.

II. EXTENDED THERMODYNAMICS

Extended thermodynamics can be based on the kinetic theory of monatomic ideal gases. The set of variables is defined by moments of the distribution function f. The equations of transfer for those moments are developed from the Boltzmann equation and the closure problem is solved by maximizing the entropy [7,8]. The first 13 variables have an easy physical interpretation. These are the density ρ, velocity v_i, temperature T, pressure deviator $p_{\langle ij\rangle}$ (where the angular brackets denote the symmetric traceless part), and the heat flux q_i. Here, the linearized equations that follow from the entropy maximization are equivalent to Grad's 13-moment theory [3,8]. If we add to the first 13 variables the full traceless part $m_{\langle ijk\rangle}$ of the third moment (7 components) and the nonequilibrium part Δ of the full trace of the fourth moment, we get a system with 21 moments. If we consider a steady state problem in which all variables depend only on one space dimension x, this system reduces to seven equations. With σ for $p_{\langle 11\rangle}$, q for q_1, and m for $m_{\langle 111\rangle}$, we have

$$\frac{d}{dx}\{\rho v\}=0, \tag{1}$$

$$\frac{d}{dx}\{\rho v^2+\rho RT+\sigma\}=0, \tag{2}$$

$$\frac{d}{dx}\{\rho v^3+5\rho RTv+2\sigma v+2q\}=0, \tag{3}$$

$$\frac{d}{dx}\left\{\frac{2}{3}\rho v^3+\left(\frac{4}{3}\rho RT+\frac{7}{3}\sigma\right)v+\frac{8}{15}q+m\right\}=-\alpha\rho\sigma, \tag{4}$$

$$\frac{d}{dx}\left\{\frac{1}{2}\rho v^4+\left(4\rho RT+\frac{5}{2}\sigma\right)v^2+\left(\frac{16}{5}q+m\right)v+\frac{5}{2}\rho R^2T^2+\frac{7}{2}RT\sigma+\frac{1}{6}\Delta\right\}=-\alpha\rho\left(\sigma v+\frac{2}{3}q\right), \tag{5}$$

$$\frac{d}{dx}\left\{\frac{2}{5}\rho v^4+\left(\frac{6}{5}\rho RT+3\sigma\right)v^2+\left(\frac{24}{25}q+\frac{14}{5}m\right)v+\frac{9}{5}RT\sigma\right\}=-\alpha\rho\left(\frac{9}{5}\sigma v+\frac{3}{2}m\right), \tag{6}$$

$$\frac{d}{dx}\left\{\rho v^5+(14\rho RT+8\sigma)v^3+\left(\frac{84}{5}q+4m\right)v^2+\left(35\rho R^2T^2+28RT\sigma+\frac{7}{3}\Delta\right)v+28RTq\right\}=-\alpha\rho\left(4\sigma v^2+\frac{16}{3}qv+\frac{2}{3}\Delta\right). \tag{7}$$

R denotes the gas constant and α is a constant that follows by calculation of the collision production for Maxwell molecules. The first three equations are the equations of balance for the conserved quantities mass, momentum, and energy. If we neglect the last equation (7) and set $\Delta=0$, we get six equations, which represent the stationary one-dimensional case of extended thermodynamics with 20 variables. Neglecting Eq. (6) and setting $m=0$, we get the 14-moment theory. Neglecting Eqs. (6) and (7) and setting $m=0$ and $\Delta=0$, we get Grad's 13-moment theory.

The necessary number of variables depends on the considered experiment. A satisfactory description of experiments of light scattering and dispersion relation of sound waves needs hundreds of variables [8,9] under certain circumstances.

III. SINGULAR POINTS IN A STEADY STATE SHOCK STRUCTURE

For simplicity we consider a steady state shock. At point x_0, very far before the shock, we have the equilibrium state ρ_0, v_0, T_0 and on the other side, very far behind the shock at point x_1, we have the equilibrium state ρ_1, v_1, T_1. All other quantities σ, q, m, and Δ are zero at both points. The adiabatic speed of sound at the points x_0 and x_1 is given by $a_0=\sqrt{(5/3)RT_0}$ and $a_1=\sqrt{(5/3)RT_1}$, respectively. We introduce the Mach number at x_0 by $M_0=v_0/a_0$. The integration of Eqs. (1)–(3) between x_0 and x_1 leads to the Rankine-Hugoniot-relations

$$\rho_1=\frac{4M_0^2}{M_0^2+3}\rho_0, \tag{8a}$$

$$v_1=\frac{M_0^2+3}{4M_0^2}v_0, \tag{8b}$$

$$T_1=\frac{5M_0^4+14M_0^2-3}{16M_0^2}T_0. \tag{9}$$

The shock structure between the points x_0 and x_1 can now be calculated by one of the systems above, with 13, 14, 20, or 21 moments. Let $\mathbf{u}$ denote the vector of variables $\mathbf{u}=\{\rho,v,T,\sigma,q,\dots\}$, then all systems may be written in the form

$$\frac{d\mathbf{f}(\mathbf{u})}{dx}=\mathbf{r}(\mathbf{u}). \tag{10}$$

$\mathbf{f}(\mathbf{u})$ denotes the fluxes and $\mathbf{r}(\mathbf{u})$ denotes the right hand sides of the system (1)–(7). Differentiating the fluxes with respect to $\mathbf{u}$ and introducing the matrix $\mathbf{A}(\mathbf{u})=\partial\mathbf{f}(\mathbf{u})/\partial\mathbf{u}$ we get

$$\mathbf{A}(\mathbf{u})\cdot\frac{d\mathbf{u}}{dx}=\mathbf{r}(\mathbf{u}). \tag{11}$$

This is a linear system for the vector of derivatives $d\mathbf{u}/dx$. The solution of the system depends strongly on the structure of $\mathbf{A}(\mathbf{u})$ and $\mathbf{r}(\mathbf{u})$. At the points x_0 and x_1 the productions $\mathbf{r}(\mathbf{u})$ vanish, but between x_0 and x_1 they do not vanish in general. Therefore the system (11) is inhomogenous in general and there is a problem, if the determinant of $\mathbf{A}(\mathbf{u})$ vanishes. By Cramer's rule the system (11) may be solved for the vector of derivatives. The solution may be represented schematically as

$$\frac{d\mathbf{u}}{dx}=\frac{\mathbf{z}}{D}. \tag{12}$$

D is the determinant of $\mathbf{A}$ and the kth component of $\mathbf{z}$ is a determinant obtained from $\mathbf{A}$ by replacing its kth column by $\mathbf{r}$.

At the points x_0 and x_1 the determinant D of $\mathbf{A}(\mathbf{u})$ is zero, if the velocity v is equal to a characteristic velocity c. For example, in the 14-moment case we have

$$D_0=\det\{\mathbf{A}(\mathbf{u}_0)\}=0 \quad \text{if } v_0=\begin{cases} c_0^{(1)}=0.900a_0 \\ c_0^{(2)}=1.763a_0, \end{cases} \tag{13}$$

$$D_1=\det\{\mathbf{A}(\mathbf{u}_1)\}=0 \quad \text{if } v_1=\begin{cases} c_1^{(1)}=0.900a_1 \\ c_1^{(2)}=1.763a_1. \end{cases} \tag{14}$$

We see that at x_0 we get a problem, if M_0 is equal to 0.9 or 1.763. Now we look behind the shock, at the point x_1. By (9) we may write a relation between the characteristic velocities at x_0 and x_1,

$$c_1=\left(\frac{5M_0^4+14M_0^2-3}{16M_0^2}\right)^{1/2}c_0. \tag{15}$$

We ask for the Mach number M_0 at which at the point x_1 the velocity v_1 equals a characteristic velocity c_1. We set c_1 equal to v_1 which is given by (8b), and get

$$M_0=\left(\frac{3a_0^2+c_0^2}{5c_0^2-a_0^2}\right)^{1/2}. \tag{16}$$

For the two characteristic velocities (13) in the 14-moment case we get $M_0=0.648$ and $M_0=1.117$. At these two Mach numbers the velocity v_1 is equal to $c_1^{(1)}$ or $c_1^{(2)}$. If we increase the Mach number, starting at $M_0=1$, we see that in the 14-moment theory the problem $\det(\mathbf{A})=0$ occurs first at $M_0=1.117$ at the point x_1. Inspection of the determinants shows, that for M_0 not much above 1.117, D_0 is negative and D_1 is positive. Therefore the point at which the determinant D vanishes moves from point x_1—where it is located for $M_0=1.117$—in the direction of x_0 when M_0 is increased. We conclude: in the 14-moment theory we have a singular point at $x_0<x<x_1$ for $M_0>1.117$. For $M_0=1.763$ we get a second singular point at x_0. Increasing the Mach number, this second singularity moves from x_0 in the direction of x_1. But there is a significant difference between these two singular points. By the numerical calculations below, we see that the singularity starting at $M_0=1.117$ is a regular singular point, so that the numerator $\mathbf{z}$ in (12) also vanishes. The singularity arising at $M_0=1.763$ is a regular singular point, but for M_0 a little bit greater than 1.763 this point moves into the shock and becomes an irregular singular point, in which $\mathbf{z}$ does not vanish. We have $\mathbf{r}\neq 0$, $\mathbf{z}\neq 0$, and $D=0$, hence the derivatives go to infinity. Therefore, a continuous shock structure exists up to the critical Mach number $M_0=1.763$.

TABLE I. Mach numbers for $D_0=0$ and $D_1=0$.

Moments	$D_0=0$, for	$D_1=0$, for
13	$M_0=\begin{cases}0.629\\1.650\end{cases}$	$M_0=\begin{cases}0.673\\1.859\end{cases}$
14	$M_0=\begin{cases}0.9\\1.763\end{cases}$	$M_0=\begin{cases}0.648\\1.117\end{cases}$
20	$M_0=\begin{cases}0.574\\0.774\\1.808\end{cases}$	$M_0=\begin{cases}0.639\\1.341\\2.260\end{cases}$
21	$M_0=\begin{cases}0.644\\1.010\\1.887\end{cases}$	$M_0=\begin{cases}0.624\\0.989\\1.780\end{cases}$

The number of characteristic velocities and the value of the Mach numbers at which D_0 and D_1 vanish may be read off from Table I for several theories.

IV. NUMERICAL CALCULATION OF THE SHOCK STRUCTURE

Usually the problem is solved as an initial value problem [1,4]. But this procedure leads to difficulties at the regular singular points. Therefore, we consider the problem as a boundary value problem. The numerical scheme is based on the system (10). The derivative of $\mathbf{f}$ with respect to x is approximated by central differences. This system is written down for discrete points x^i with $x_0 \leqslant x^i \leqslant x_1$. This leads to a nonlinear algebraic system for the variables $\mathbf{u}(x^i)$, which can be solved if the boundary values at the finite points x_0 and x_1 are known. The Rankine-Hugoniot relations connect the values $\mathbf{u}$ at infinity far before and at infinity far behind the shock. If the interval x_1-x_0 is chosen large enough, the deviation of $\mathbf{u}$ at the points x_0 and x_1 from the Rankine-Hugoniot values is lower than the chosen precision 10^{-6} of the solver for the nonlinear system. This is proved by variation of the interval x_1-x_0. Therefore, we can take the Rankine-Hugoniot values as the necessary boundary values at x_0 and x_1. We introduce dimensionless variables by

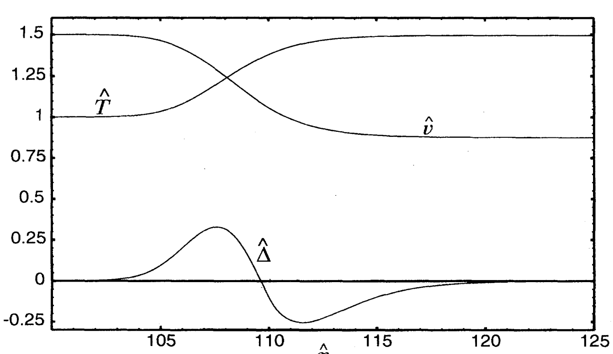

FIG. 1. Shock structure in the 14-moment theory for $M_0=1.5$.

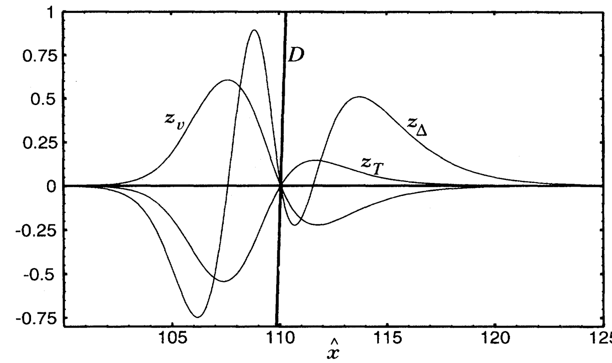

FIG. 2. Main determinant and numerators in the 14-moment theory for $M_0=1.5$.

$$\hat{x}=\frac{\rho_0\alpha}{a_0}x,\quad \hat{\rho}=\frac{\rho}{\rho_0},\quad \hat{v}=\frac{v}{v_0},\quad \hat{T}=\frac{T}{T_0},\quad \hat{\sigma}=\frac{\sigma}{\rho_0 R T_0},\tag{17}$$

$$\hat{q}=\frac{q}{\rho_0 R T_0 a_0},\quad \hat{m}=\frac{m}{\rho_0 R T_0 a_0},\quad \hat{\Delta}=\frac{\Delta}{\rho_0 R T_0 a_0^2}.\tag{18}$$

From (1), (2), and (3) and the Rankine-Hugoniot relations we may derive equations for $\hat{\rho}$, $\hat{\sigma}$, and $\hat{q}$:

$$\hat{\rho}=\frac{M_0}{\hat{v}},\quad \hat{\sigma}=M_0\left\{\frac{5}{3}(M_0-\hat{v})-\frac{\hat{T}}{\hat{v}}\right\}+1,\tag{19}$$

$$\hat{q}=\frac{M_0}{2}\left\{\frac{5}{3}(M_0-\hat{v})^2-3\hat{T}+5\right\}-\hat{v}.\tag{20}$$

We start with the 13-moment theory. By elimination of $\hat{\rho}$, $\hat{\sigma}$, and $\hat{q}$ with (19) and (20) we obtain a system for the variables $\mathbf{u}=\{\hat{v},\hat{T}\}$. The numerical solution of this system leads to the well known [4,5] continuous shock structure up to $M_0=1.65$. Then an irregular singular point occurs at x_0 and no continuous shock exists for $M_0>1.65$. There is no other singularity for $1\leqslant M_0<1.65$ in the 13-moment theory.

Next we consider the 14-moment theory. With (19) and (20) the vector of the variables is $\mathbf{u}=\{\hat{v},\hat{T},\hat{\Delta}\}$. The numerical solution of this system, in the form of (10), for $M_0=1.5$ is shown in Fig. 1. If we write down the system in the form (12), then the numerator contains three elements:

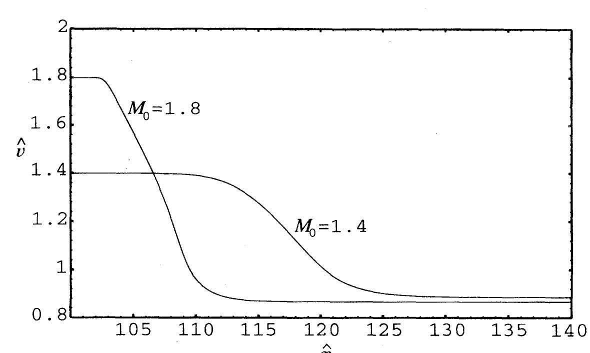

FIG. 3. Velocity in the 21-moment theory.

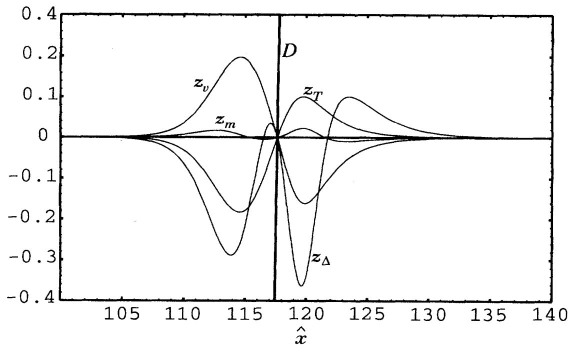

FIG. 4. Main determinant and numerators in the 21-moment theory for $M_0 = 1.4$.

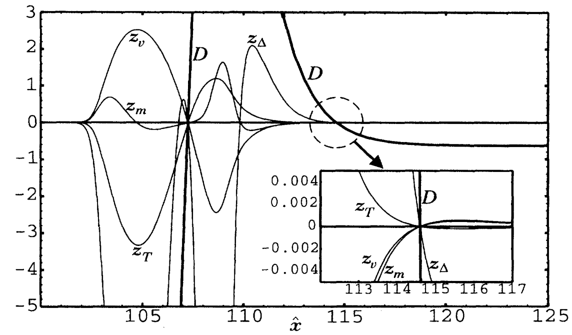

FIG. 5. Main determinant and numerators in the 21-moment theory for $M_0 = 1.8$.

$\mathbf{z} = \{z_v, z_T, z_\Delta\}$. These three modified determinants and the main determinant D are shown in Fig. 2. We see that at the point $x = 110.05$ at which the determinant D vanishes all numerators vanish as well. The numerical calculations show that this is always the case for $M_0 < 1.763$. For $M_0 > 1.763$ no continuous shock structure exists.

In the 20-moment theory we have $\mathbf{u} = \{\hat{v}, \hat{T}, \hat{m}\}$. The numerical solutions are qualitatively the same as in the 14-moment theory. A regular singular point arises for $M_0 > 1.341$, starting at x_1. For $M_0 > 1.808$ an irregular singular point arises, starting at x_0. Therefore a continuous shock structure exists for $M_0 < 1.808$.

Finally we consider the 21-moment theory. The vector of the variables is given by $\mathbf{u} = \{\hat{v}, \hat{T}, \hat{m}, \hat{\Delta}\}$. A singularity arises at the first time at $M_0 = 1.01$ at the point x_0 before the shock. For $M_0 = 1.4$ the singularity has moved into the shock and can be found at $x = 117.63$. The singularity is regular and the continuous shock structure is shown in Fig. 3. In Fig. 4 we see that all numerators vanish when the main determinant vanishes. For $M_0 = 1.78$ a second regular singularity arises at x_1 behind the shock. For $M_0 = 1.8$ this singular point has moved into the shock and can be found at $x = 114.6$. The singularity that comes from the point x_0 is now at $x = 107.25$. The continuous shock structure for $M_0 = 1.8$ is also shown in Fig. 3. In Fig. 5 we can see that at both singular points all determinants vanish. If M_0 equals 1.887, an irregular singular point arises at x_0 and no continuous shock structure exists. Therefore a continuous shock structure exists for $M_0 < 1.808$.

V. CONCLUSIONS

The numerical calculations for extended thermodynamics of 13, 14, 20, and 21 moments have shown that in all theories a continuous shock structure exists up to the *biggest* characteristic velocity at x_0 in front of the shock. All singular points that arise before the biggest characteristic velocity is reached are regular singularities. This observation has a simple physical interpretation. If the velocity of the gas in front of the shock is higher than the biggest characteristic velocity, no signal can reach the shock and therefore no continuous shock is possible. In extended thermodynamics the biggest characteristic velocity increases by increasing the number of moments [8]. Therefore, it should be possible to calculate continuous shock structures for high Mach numbers.

[1] D. Gilbarg, and D. Paolucci, J. Rat. Mech. Anal. **2**, 617 (1953).
[2] H. Grad, Commun. Pure Appl. Math. **5**, 257 (1952).
[3] H. Grad, in *Thermodynamics of Gases*, Handbuch der Physik Vol. 12, edited by S. Flügge (Springer-Verlag Berlin, 1958).
[4] A. M. Anile and A. Majorana, Meccanica **16**, 149 (1981).
[5] D. Jou and D. Pavón, Phys. Rev. A **44**, 6496 (1991).
[6] T. Ruggeri, Phys. Rev. E **47**, 4135 (1993).
[7] W. Dreyer, J. Phys. A: Math. Gen. **20**, (1987).
[8] I. Müller and T. Ruggeri, *Extended Thermodynamics*, Springer Tracts on Natural Philosophy Vol. 37 (Springer-Verlag, New York, 1993).
[9] W. Weiss and I. Müller, Continuum Mech. Thermodyn. **7**, 1 (1995).