Burnett Description of Strong Shock Waves

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In 1992 Salomons and Mareschal [Phys. Rev. Lett. **69**, 269 (1992)] gave evidence that the Burnett equations can provide an important improvement over the Navier-Stokes equations for shock waves at high Mach numbers. In this Letter we solve the Burnett equations and make a comparison with the results from molecular dynamics, the Navier-Stokes equations, and the theory advanced by Holian *et al.* [Phys. Rev. E **47**, R24 (1993)]. A qualitative analysis of the Burnett equations is also done and some open problems are mentioned. [S0031-9007(98)07042-2]

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Shock waves appear in a variety of physical phenomena [1,2], in which the main characteristic is the large values of the state variables and their drastic changes within small distances, typically of the order of a few mean free paths. Recently, they have been used to propose an explanation for the sonoluminescence phenomena [3]. They also provide a natural arena in which different theories can stringently be tested. The Navier-Stokes equations can be used to provide a description for several shock wave propagation phenomena, and while they describe some of the features, the description is subject to improvement, especially for strong shocks. Among the theories that extend the Navier-Stokes description is the one provided by the Burnett constitutive equations obtained by Chapman and Cowling [4], and it is our goal to see up to what point the Burnett description is adequate for describing shock wave profiles. We also point out the main mathematical problems for such a description to be valid. Since even for the Navier-Stokes equations solutions in closed form are not known, we have used numerical methods to study the Burnett equations. We would like to emphasize that we are using numerical methods because in nonlinear phenomena it is rather often the only way to go. Nevertheless, numerical methods are in general not enough to achieve a proper understanding of the underlying dynamics of the differential equations so that we have complemented them by a qualitative analysis of the dynamical system provided by the Burnett equations.

In 1992 Salomons and Mareschal [5] gave convincing evidence that the Burnett equations provide an important improvement over the Navier-Stokes equations for strong shock waves, although they did not obtain the velocity and temperature profiles. Here we will go one step further and obtain both profiles using the Burnett equations for the situation reported by Holian *et al.* [6].

The Burnett corrections to the pressure tensor and the heat flux were taken from Chap. 15 of the book by Chapman and Cowling [4] for the case of a stationary plane shock wave which moves along the x axis with velocity $u(x)$. The coefficients (ω's and θ's) that appear in the expressions for the pressure tensor and the heat flux [see Eqs. (15.3,8) and (15.3,6) in the book by Chapman and Cowling [4] and Eq. (1) below] correspond to the ones calculated by Burnett [4] and by Wang-Chang and Uhlenbeck [7] for the rigid sphere case using the first order Sonine expansion for the viscosity [6]. Our calculations for the Burnett corrections of the fluxes are in agreement with the ones reported by Wang-Chang [7] except for a numerical factor which multiplies ω_6 in his expression for the pressure tensor. It is important to point out that the general form of these equations can be obtained using strictly a macroscopic reasoning [8]. Adopting the same dimensionless variables as Holian *et al.* [6], the calculated Burnett corrections for the xx component of the reduced stress tensor and the x component of the heat flux are given by

$$\mathbf{P}_{xx}^{\star(2)} \equiv \frac{\mathbf{P}_{xx}^{(2)}}{\rho_0 u_0^2} = \left\{ [2\,\omega_1/3 - 14\,\omega_2/9 + 2\,\omega_6/9]\left(\frac{du^\star}{ds}\right)^2 - \frac{2}{3}\,\omega_2\,\frac{d}{ds}\left[u^\star \frac{d}{ds}(\tau/u^\star)\right] + \frac{2}{3}\,\omega_3\,\frac{d^2\tau}{ds^2} + \frac{2}{3}\,\omega_4\,\frac{u^\star}{\tau}\,\frac{d}{ds}(\tau/u^\star)\,\frac{d\tau}{ds} + \frac{2}{3}\,\frac{\omega_5}{\tau}\left(\frac{d\tau}{ds}\right)^2 \right\} \frac{9\,u^\star}{16},$$

$$\mathbf{q}_{x}^{\star(2)} \equiv \frac{\mathbf{q}_{x}^{(2)}}{\rho_0 u_0^3} = \left\{ [\theta_1 - 8\,\theta_2/3 + 2\,\theta_5]\left(\frac{du^\star}{ds}\right)\left(\frac{d\tau}{ds}\right) + \frac{2}{3}\,[\theta_4 - \theta_2]\tau\,\frac{d^2u^\star}{ds^2} + \frac{2\,\theta_3 u^\star}{3}\,\frac{du^\star}{ds}\,\frac{d}{ds}(\tau/u^\star) \right\} \frac{9\,u^\star}{16}, \tag{1}$$

where ρ_0 and u_0 are the mass density and velocity at the low density region of the shock wave, respectively. Here $u^\star \equiv u/u_0$ is the reduced velocity, $\tau \equiv kT/mu_0^2$ is a reduced temperature, and s is equal to x/l, with l the "mean free path" as defined by Holian *et al.* [6]. In terms of the previous dimensionless variables the Rankine-Hugoniot jump

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conditions give for the reduced variables at the high density part of the shock ($u_1^\star$,τ_1) the following parametrization in terms of τ_0, $u_1^\star = \frac{5}{4}\tau_0 + \frac{1}{4}$, $\tau_1 = \frac{7}{8}\tau_0 + \frac{3}{16} - \frac{5}{16}\tau_0^2$, where $u_0^\star = 1$ always. Furthermore defining the Mach number (M_a) as the ratio of the shock velocity divided by the sound velocity, both velocities evaluated at the low density part of the shock, it turns out that for a monatomic gas for which the ratio of the specific heat at constant pressure divided by the one at constant volume is equal to $5/3$, we obtain that $M_a = \sqrt{0.6/\tau_0}$.

Substitution of the complete xx component of the pressure tensor, meaning the Navier-Stokes [6] plus the Burnett contributions, and the x component of the heat flux into the integrated form of the reduced conservation equations for momentum and energy [6], leads us to obtain two second order differential equations for $u^\star$ and τ. Such a second order system can be written as a first order one in four dimensions for the variables $y_1(s) = u^\star(s)$, $y_2(s) = \tau(s)$, $y_3(s) = u^{\star\prime}(s)$, and $y_4(s) = \tau'(s)$, where a prime denotes the derivative with respect to s. The system is of the form $\mathbf{y}' = \mathbf{F}(\mathbf{y}, \tau_0)$, where $\mathbf{F}_1(\mathbf{y}, \tau_0) = y_3$, $\mathbf{F}_2(\mathbf{y}, \boldsymbol{\tau}_0) = y_4$,

$$\mathbf{F}_3 = \frac{3}{2\,y_1^2\,y_2(\theta_4 - \theta_2)}\left[\frac{40}{9}\tau_0\,y_1 - \frac{16}{9}\tau_0\,y_1^2 + \frac{8}{9}\,y_1 - \frac{16}{9}\,y_1^2 + \frac{8}{9}\,y_1^3 - \frac{8}{3}\,y_1\,y_2 + 5\,y_1\,y_4\sqrt{y_2} - y_3\,y_4\,y_1^2 \times\left(\theta_1 - \frac{8}{3}\,\theta_2 + \frac{2}{3}\,\theta_3 + 2\,\theta_5\right) + \frac{2}{3}\,y_1\,\theta_3\,y_3^2\,y_2\right],$$

$$\mathbf{F}_4 = \frac{1}{y_1^2\,y_2\,(c_2 + c_3)}\left[\frac{16}{9}\tau_0\,y_1\,y_2 + \frac{16}{9}\,y_1\,y_2 - \frac{16}{9}\,y_1^2\,y_2 - \frac{16}{9}\,y_2^2 + \frac{16}{9}\,y_1\,y_2^{3/2}\,y_3 + y_1\,y_2^2\,c_2\,\mathbf{F}_3(\mathbf{y}, \tau_0) - y_3^2\,(y_1^2\,y_2\,c_1 + y_2^2\,c_2) - y_4^2\,y_1^2\,(c_4 + c_5) + y_3\,y_4\,y_1\,y_2\,(c_2 + c_4)\right], \tag{2}$$

and $c_1 = \frac{2}{3}\omega_1 - \frac{14}{9}\omega_2 + \frac{2}{9}\omega_6$, $c_2 = -\frac{2}{3}\omega_2$, $c_3 = \frac{2}{3}\omega_3$, $c_4 = \frac{2}{3}\omega_4$, and $c_5 = \frac{2}{3}\omega_5$. Finally the coefficients ω's and θ's are given by

$$\omega_1 = 1.014 \times 4, \qquad \omega_2 = 1.014 \times 2,$$
$$\omega_3 = 0.806 \times 3, \qquad \omega_4 = 0.681,$$
$$\omega_5 = \tfrac{3}{2} \times 0.806 - 0.99, \qquad \omega_6 = 0.928 \times 8,$$
$$\theta_1 = \tfrac{45}{4} \times 1.035, \qquad \theta_2 = \tfrac{45}{8} \times 1.035,$$
$$\theta_3 = -3 \times 1.03, \qquad \theta_4 = 3 \times 0.806,$$
$$\theta_5 = 8.3855. \tag{3}$$

If U denotes the open set $(0,\infty) \times (0,\infty) \times R \times R$, R being the set of real numbers, we see that, for fixed τ_0, $\mathbf{F}(\cdot, \tau_0)$ has continuous partial derivatives of any order in U. The mathematical problem posed by the shock wave problem in the Burnett regime is to find, for a fixed Mach number (fixed τ_0), a heteroclinic trajectory of $\mathbf{y}' = \mathbf{F}(\mathbf{y}, \tau_o)$ which joins the two critical points $\mathbf{y}^{\text{up}} = (1, \tau_0, 0, 0)$ and $\mathbf{y}^{\text{down}} = (u_1^\star, \tau_1, 0, 0)$ which is equivalent to posing a boundary value problem.

The Mach number for which the molecular dynamics (MD) calculations were reported is equal to 134 [5], for this value $\tau_0 \approx 3 \times 10^{-5}$, and we will take as an approximation $\tau_0 = 0$. Such an approximation is not essential and was chosen in order to compare with previous calculations by Holian *et al.* [6]. In fact, shock wave profiles can be generated for all Mach numbers but due to the lack of space our calculations will not be reported. It must be pointed out that for low Mach numbers strong evidence that the Burnett equations provide a better description than the Navier-Stokes equations has been given [9]. Following other authors [6,10] we approximate the previous boundary value problem by an initial value one, using the initial values; $u^\star(s_i) = 0.250\,006$, $\tau(s_i) = 3/16$ [6]. On the other hand, the initial values for the derivatives were taken to be zero. The initial value of s_i was determined in such a way that the numerical solution gives $u^\star(0) = 0.625$ according to the choice of the origin [6]. Two explicit numerical methods are used to solve the differential equations (2), the Adams' method and the backward differentiation formula (BDF) as implemented by the Numerical Algorithms Group FORTRAN library. The results of both methods are practically indistinguishable and can be read in Figs. 1 and 2 where (MD) calculations [5,6], the theory advanced by Holian *et al.* [6], and the Navier-Stokes are also exhibited.

It is found that the numerical solution cannot be obtained for values of s lower than about -1.5 for the Navier-Stokes equations, -2.1 for the Holian *et al.* equations, and about $s = -2$ for the Burnett equations. However, the reason for this is different in the case of the Burnett equations when compared to the Navier-Stokes and Holian *et al.* equations. In fact, for $\tau_0 > 0$ we can obtain numerical solutions for the latter equations in a wide range of values for s, and this is a result of taking $M_a = \infty$ ($\tau_0 = 0$). The general methodology of perturbing the downstream critical point by making the velocity slightly greater and integrating upstream, which we refer to as integrating in the negative direction, is a robust one in the sense that the profiles for finite Mach numbers can be obtained in this way. This works for the three theories considered here. Our explanation for this to occur is that the initial point is in the basin of attraction, $s \to -\infty$, of an invariant set that turns out to be the solution sought. However, in the case of the Burnett equations the existence of a heteroclinic trajectory is not clear for all Mach numbers as we now argue.

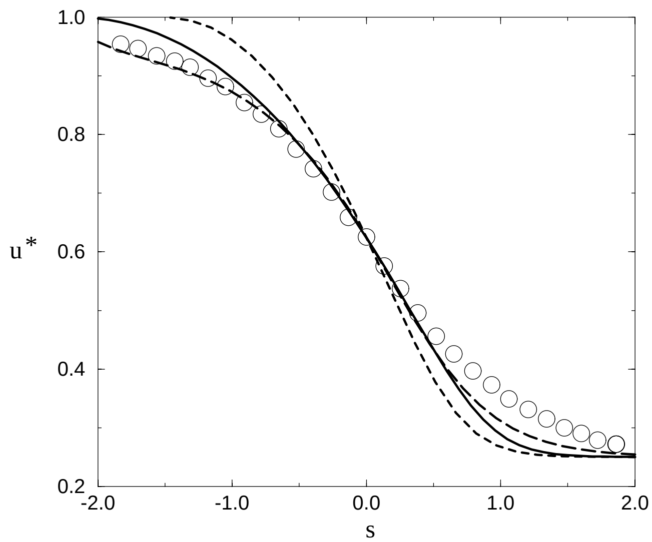

FIG. 1. Reduced velocity profiles $u^\star$ vs s. Circles: molecular dynamics ($M_a = 134$); solid line: theory by Holian *et al.* ($\tau_0 = 0$); dashed line: Navier-Stokes ($\tau_0 = 0$); and long-dashed line: Burnett ($\tau_0 = 0$).

The eigenvalues (λ) of the differential of $\mathbf{F}$ at $\mathbf{y}^{\rm up}$ $[\mathbf{F}'(\mathbf{y}^{\rm up})]$ can be seen to be roots of the equation

$$54\tau_0^{5/2}(\theta_2 - \theta_4)\,(c_2 + c_3)\,\lambda^4 + 405\,\tau_0^3\,c_2\,\lambda^3 + \tau_0^{5/2}[96\,(\theta_2 - \theta_4) - 360\,c_2 - 144\,c_3]\lambda^2 + \tau_0^2(720\,\tau_0 - 1104)\lambda + \tau_0^{3/2}(384 - 640\,\tau_o) = 0\,. \quad (4)$$

It is easily seen that for $M_a = 1$ ($\tau_0 = 3/5$) $\lambda = 0$ is a solution with multiplicity one, so for $M_a = 1$, $\mathbf{y}^{\rm up} = \mathbf{y}^{\rm down}$ is a nonhyperbolic point. For $M_c > M_a > 1$ ($M_c \approx 2.6899$) we found that the eigenvalues are complex and all have a positive real part; for $M_a = M_c$ two eigenvalues have zero real part, and for $M_a > M_c$ the eigenvalues are complex: two of them have positive real parts, and the other two have negative real parts. In brief, for $M_a = 1, M_c$, the upstream critical point is not hyperbolic, for $M_c > M_a > 1$ the upstream critical point is an unstable node, and for $M_a > M_c$ the upstream critical point is a saddle. For the other critical point it is found that for $M_a > 1$ the eigenvalues of $\mathbf{F}'(\mathbf{y}^{\rm down})$ are all real, three of them are positive, and one is negative. So for $M_a > 1$ the downstream critical point is a saddle.

The Hartman-Grobman theorem [11] establishes that the local qualitative behavior of the linearized differential equations and the nonlinear ones is the same for hyperbolic critical points. Since for $M_a \neq 1$ and $M_a \neq M_c$ the eigenvalues at the upstream critical point are complex we infer that the behavior of the solution near $\mathbf{y}^{\rm up}$ is oscillatory. This fact could be advanced as an argument to invalidate the Burnett description since for shock waves a monotonic profile is expected. However, this is a short sighted argument since for $M_a < M_c$ the oscillations are irrelevant. Nevertheless, as the Mach number is increased ($M_a > M_c$) the oscillations grow instead of decreasing, for $M_c < M_a < M_{c1}$ ($M_{c1} \approx 3.25$) the numerical solution remains bounded, and for larger Mach numbers the numerical solution cannot be obtained for lower values of s than a certain negative value of s $[s_c(\tau_0)]$. We have evaluated the eigenvectors at the critical upstream point for $M_a = 2.8$. When we perturb the upstream critical point along the eigenvectors corresponding to the unstable manifold and integrate in the negative direction, we found that the numerical solution does not go to the critical point but exhibits an oscillatory behavior. In other words, there is evidence of an attracting region. We have used the reconstruction technique for attractors [12], which is based on a remarkable result by Takens, and found that the attracting region is a limit cycle; see Fig. 3. What happens for

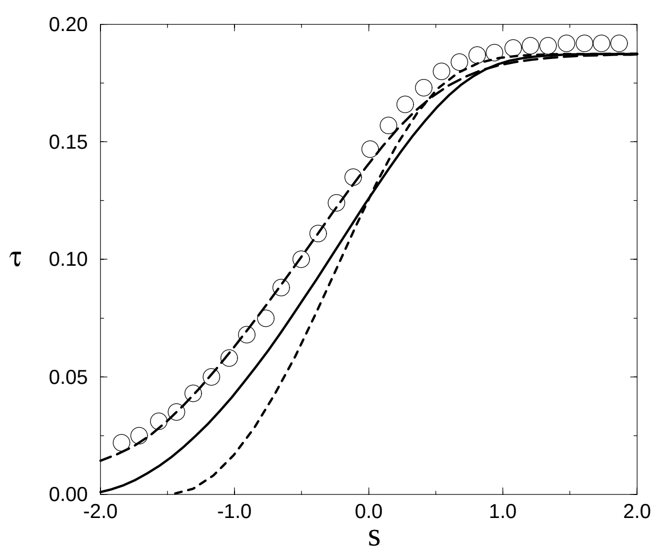

FIG. 2. Reduced temperature profiles τ vs s. The meaning of the symbols and lines is as in Fig. 1. $\tau_0 = 0$.

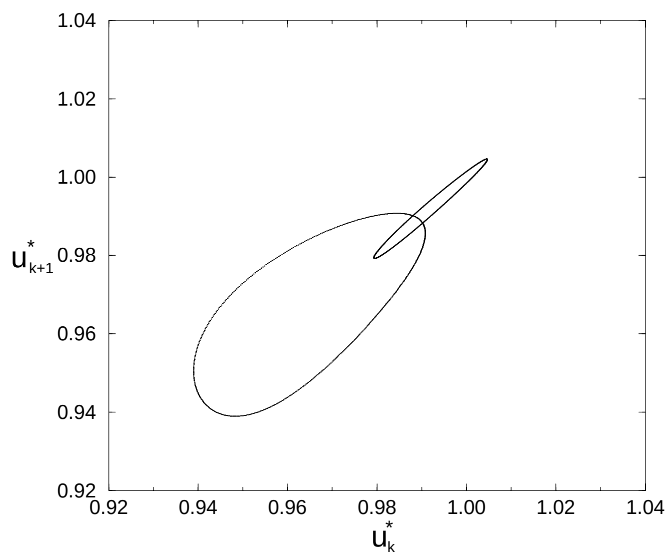

FIG. 3. Long time behavior, k large, of the numerical solution at equal spaced points $s_k = s_i + k\Delta$, $u_k^\star \equiv u^\star(s_k)$. The larger and wider limit cycle corresponds to $M_a = 3.1$ and the other one to $M_a = 2.8$.

$M_a > M_{c1}$ is that the limit cycle has grown large enough to touch a repelling region. So, when the unstable node becomes a saddle there appears a limit cycle which eventually, as the Mach number is increased, disappears. This may be considered as an indication that a heteroclinic trajectory does not exist for $M_a > M_c$. It is interesting to notice that there are some similarities of the bifurcation just described at $M_a = M_c$ and the Hopf bifurcation [11].

We must not forget that we are interested in a heteroclinic trajectory, and this is the subject of global analysis. The condition for the existence of a heteroclinic trajectory [13] is that the stable manifold of one critical point intersects in a smooth way the unstable manifold of the other; for hyperbolic critical points the existence of such manifolds is guaranteed by the stable manifold theorem [11]. Montgomery [14] has given some conditions that assure that the Burnett equations, and the higher order gradient Chapman-Enskog expansions, have a heteroclinic trajectory for Mach numbers near and above 1 although the explicit upper limit is not known. These conditions can be shown to be satisfied by the equations considered in this work so that the Burnett equations have a shock structure at least for Mach numbers near one. Our calculations suggest that the upper limit is M_c, and we have obtained numerical solutions with structure for slightly higher numbers than M_c, but the limit cycle is probably so small that it cannot be resolved. It is interesting to notice that the change in the Conley index at M_c for the upstream critical point implies the existence of a nonconstant solution contained in a compact set (see Ref. [13], p. 456). If such a solution could be shown to be gradientlike, then, according to Montgomery [14], a heteroclinic trajectory exists.

Coming back to the numerical results given in Figs. 1 and 2, we see that the numerical solution cannot be found for values of s lower than about -2 because the local flow associated with the differential equation, for the initial conditions used, cannot be extended to $s = -\infty$. In such a case the behavior of the numerical solution, for $M_a > M_{c1}$, seems to be consistent with the theoretical results in Hirsh and Smale [15]. What is remarkable is that the piece of the invariant set that remains is in good agreement with MD calculations. However, the results from MD are also restrictive [6]. Indeed, two facts may be observed [5,16]. One is that the data exhibit dispersion and second that they exhibit oscillatory type behavior for the profiles which is also found in some raw data generated by the direct simulation Monte Carlo method [5,9]. So, one may question if such a dispersion and oscillatory type behavior may be an indication that a shock structure does not exist.

On the other hand, the Navier-Stokes equations have a structure for high Mach numbers, but it must be pointed out that this does not mean that the solution can be observed. In order to be observed the solution must be stable in the hydrodynamic sense [17] which poses a difficult mathematical problem even in its linearized version which unfortunately is in general not conclusive. In this respect it is important to mention that a linearized hydrodynamic stability analysis has been carried out for the constant solutions to the Euler equations for certain normal modes [2]. The consideration of the viscous case would possibly provide a bound to the Mach number for which the solution to the Navier-Stokes equations, or to the Burnett equations, ceases to be stable, but this interesting problem would lead us too far from the objective of this work.

The results given here show that the Burnett equations are on the right track to provide a better description for shock waves so it is then natural to think that the super-Burnett and higher order gradient expansions may enlarge the domain of Mach's numbers for which an heteroclinic curve exists. However, such expansions are rather difficult to deal with and have some problems so it seems better to look for other alternatives but this is a subject for further work.

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