Shock waves in a dense gas

M. López de Haro* and V. Garzó
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain
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The revised Enskog theory for a dense monatomic hard sphere gas is used to analyze the problem of shock waves. The steady profiles of velocity, density, and temperature are obtained, up to the linearized Burnett hydrodynamic order. A comparison with the results of computer simulations and of other hydrodynamic approximations is carried out.

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Strong shock waves in fluids are useful in studying far from equilibrium states. They provide a convenient way of determining thermodynamic data under extreme conditions. As a matter of fact, these waves occupy a small, rapidly moving, transition region in space that connects together two equilibrium states, namely, a relatively cold, low-pressure region to a relatively hot, high-pressure region. From a theoretical point of view and in the case of low-density gases, this problem has been extensively studied both using a continuum approach [1] as well as by means of computer simulations [2]. In particular, it is well known that plane shock waves in these systems cannot be accurately described by the Navier-Stokes equations and that the so-called Burnett equations [3] give an improvement over the Navier-Stokes predictions as compared with simulations [4,5].

The studies pertaining to dense gases are much scarcer, although they have received some attention recently. A difficulty in undertaking the continuum approach for such gases (which does not occur for a dilute gas) is the fact that, in general, the transport coefficients are not explicitly known. Nevertheless, a notable exception is the case of a hard-sphere dense gas for which the revised Enskog theory [6] represents an adequate description. In this framework, the transport coefficients have been determined up to the linearized Burnett hydrodynamic order [7]. On the other hand, the propagation of the shock wave in a dense hard-sphere gas has been numerically studied using the Enskog kinetic equation [8]. An interesting question is then whether the agreement between the predictions of the continuum approach and the simulation results observed in the low-density case is maintained for moderate densities. In this paper we will address a partial aspect of this question by analyzing the problem of planar shock waves in the context of the revised Enskog theory.

In order to describe the (one-dimensional) hydrodynamic profiles, it is convenient to consider a reference frame moving with the shock front. In this frame, the shock is fixed and achieves a steady profile due to dissipative effects. Consequently, the usual balance equations of hydrodynamics imply that

$$\rho(x)u(x) = \text{const} , \tag{1}$$

$$p(x) + \pi_{xx}(x) + \rho(x)u^2(x) = \text{const} , \tag{2}$$

$$\rho(x)[e(x) + \tfrac{1}{2}u^2(x)]u(x) + u(x)[p(x) + \pi_{xx}(x)] + q(x) = \text{const} . \tag{3}$$

Here ρ is the mass density, u is the velocity in the direction of the shock wave, p is the hydrostatic pressure, π_{xx} is the longitudinal component of the irreversible pressure tensor, e is the internal energy per mass unit, and q is the heat flux. Labeling the unshocked "cold" equilibrium state by subscript 0 and the shocked "hot" equilibrium state by subscript 1 and noting that in these two equilibrium states π_{xx} and q vanish, Eqs. (1)–(3) yield the well-known Rankine-Hugoniot conditions

$$\rho_0 u_0 = \rho_1 u_1 , \tag{4}$$

$$p_0 + \rho_0 u_0^2 = p_1 + \rho_1 u_1^2 , \tag{5}$$

$$\rho_0(e_0 + \tfrac{1}{2}u_0^2) + p_0 = \rho_1(e_1 + \tfrac{1}{2}u_1^2) + p_1 . \tag{6}$$

Thus far, both the balance equations and the Rankine-Hugoniot conditions apply for any fluid system. However, to get the profiles of density, velocity, and temperature it is necessary to specify the equation of state and the internal energy as well as the explicit expressions for the dissipative fluxes. In the context of the revised Enskog theory, the equation of state and the internal energy density for a dense monatomic hard sphere gas read, respectively,

$$p(x) = \frac{\rho(x)k_BT(x)}{m}[1 + \rho^*(x)\chi_c(x)] , \tag{7}$$

$$e(x) = \frac{3}{2}\frac{k_BT(x)}{m} , \tag{8}$$

where k_B is the Boltzmann constant, m is the mass of a molecule, χ_c is the equilibrium value of the pair correlation function at the point of contact, and $\rho^* = (2/3)(\pi\rho/m)\sigma^3$, σ being the molecular diameter. In addition, the dissipative fluxes up to the linearized Burnett order can be written as

*On leave from Laboratorio de Energía Solar, IIM-UNAM, Apartado Postal 34, Temixco 62580, Mor., Mexico.

$$\pi_{xx}(x) = -\left(\frac{4}{3}\eta(x)+\kappa(x)\right)u'(x) - \left(\alpha_1(x)-\frac{4}{3}\alpha_3(x)\right)u''(x) + \left(\alpha_2(x)+\frac{2}{3}\alpha_4(x)\right)T''(x) , \quad (9)$$

$$q(x) = -\lambda(x)T'(x) + \left(\frac{2}{3}\beta_1(x)-\beta_2(x)\right)u''(x) , \quad (10)$$

where the corresponding transport coefficients are given by [7,9]

$$\eta = \frac{\mu}{\chi_c}\left[1+\frac{4}{5}\chi_c\rho^* + \left(\frac{4}{25}+\frac{48}{25\pi}\right)(\chi_c\rho^*)^2\right] \equiv \mu g_\eta , \quad (11)$$

$$\kappa = \frac{16}{5\pi}\frac{\mu}{\chi_c}(\chi_c\rho^*)^2 \equiv \mu g_\kappa , \quad (12)$$

$$\alpha_1 = \frac{64}{25\pi}\left(\frac{\mu}{\rho\chi_c}\right)^2\left(1-\frac{37}{40}\frac{\rho^*}{\chi_c}\frac{\partial\chi_c}{\partial\rho^*}\right)(\chi_c\rho^*)^3 \equiv \left(\frac{\mu}{\rho}\right)^2 g_{\alpha_1} , \quad (13)$$

$$\alpha_2 = \frac{6}{5\pi}\frac{1}{\rho T}\left(\frac{\mu}{\chi_c}\right)^2\left(1+\frac{5}{3}\chi_c\rho^*\right)(\chi_c\rho^*)^2 \equiv \frac{\mu^2}{\rho T}g_{\alpha_2} , \quad (14)$$

$$\alpha_3 = \left(\frac{\mu}{\rho\chi_c}\right)^2\left\{1+\frac{14}{5}\chi_c\rho^*+\frac{44}{25}(\chi_c\rho^*)^2 + \left(\frac{8}{25}-\frac{192}{125\pi}\right)(\chi_c\rho^*)^3 + \left[1+\frac{4}{5}\chi_c\rho^*+\left(\frac{4}{25}+\frac{51}{125\pi}\right)(\chi_c\rho^*)^2\right]\frac{\partial\chi_c}{\partial\rho^*}\rho^{*2}\right\} \equiv \left(\frac{\mu}{\rho}\right)^2 g_{\alpha_3} , \quad (15)$$

$$\alpha_4 = \frac{1}{\rho T}\left(\frac{\mu}{\chi_c}\right)^2\left[1+\frac{6}{5}\chi_c\rho^*+\left(\frac{3}{5}+\frac{132}{25\pi}\right)(\chi_c\rho^*)^2 + \left(\frac{14}{125}+\frac{492}{125\pi}\right)(\chi_c\rho^*)^3\right] \equiv \frac{\mu^2}{\rho T}g_{\alpha_4} , \quad (16)$$

$$\lambda = \frac{15}{4}\frac{k_B\mu}{m\chi_c}\left[1+\frac{6}{5}\chi_c\rho^*+\left(\frac{9}{25}+\frac{32}{25\pi}\right)(\chi_c\rho^*)^2\right] \equiv \frac{15}{4}\frac{k_B\mu}{m}g_\lambda , \quad (17)$$

$$\beta_1 = \frac{3}{\rho}\left(\frac{\mu}{\chi_c}\right)^2\left[1+\frac{8}{5}\chi_c\rho^*+\left(\frac{21}{25}+\frac{44}{25\pi}\right)(\chi_c\rho^*)^2 + \left(\frac{18}{125}+\frac{124}{125\pi}\right)(\chi_c\rho^*)^3\right] \equiv \frac{\mu^2}{\rho}g_{\beta_1} , \quad (18)$$

$$\beta_2 = \frac{15}{4\rho}\left(\frac{\mu}{\chi_c}\right)^2\left[1+\frac{11}{5}\chi_c\rho^*+\left(\frac{39}{25}-\frac{8}{25\pi}\right)(\chi_c\rho^*)^2 + \left(\frac{9}{25}-\frac{8}{25\pi}\right)(\chi_c\rho^*)^3\right] \equiv \frac{\mu^2}{\rho}g_{\beta_2} . \quad (19)$$

Here $\mu = (5/16\sigma^2)(k_BTm/\pi)^{1/2}$ is the shear viscosity of a dilute hard-sphere gas [3] and we have introduced the auxiliary quantities g_i for later convenience. The expressions for the fluxes in the Navier-Stokes order are obtained from Eqs. (9) and (10) by dropping the terms containing u'' and T''. By substituting Eqs. (7)–(10) into the conservation equations (1)–(3) and using the jump conditions (4)–(6), one derives a closed system of nonlinear differential equations for $\rho(x)$, $u(x)$, and $T(x)$. In order to get specific results, we will consider the Carnahan-Starling approximation [10] for χ_c, namely, $\chi_c(\rho^*) = 8(\rho^*-8)/(\rho^*-4)^3$. Also, it is convenient to scale the distance x by a factor ℓ to be given below and introduce the dimensionless functions

$$\mathcal{R}(s) = \frac{\rho(x)}{\rho_0} , \quad (20)$$

$$\mathcal{U}(s) = \frac{u(x)}{u_0} , \quad (21)$$

$$\mathcal{T}(s) = \frac{k_BT(x)}{mu_0^2} , \quad (22)$$

with $s = x/\ell$. For simplicity, we choose a unit length related to the mean free path of a dilute gas of hard spheres in the cold state, namely, $\ell = (5m)/(12\rho_0\sigma^2\sqrt{\pi})$.

In terms of the above variables, the hydrodynamic equations for a steady shock wave up to the linearized Burnett order become

$$\mathcal{T}\mathcal{U}^{-1}\left(1+8\rho_0^*\mathcal{U}\frac{\rho_0^*-8\mathcal{U}}{(\rho_0^*-4\mathcal{U})^3}\right) - \left(g_\eta+\frac{3}{4}g_\kappa\right)\mathcal{T}^{1/2}\mathcal{U}' - \frac{3}{4}\left(\frac{3}{4}g_{\alpha_1}-g_{\alpha_3}\right)\mathcal{T}\mathcal{U}'' + \frac{3}{8}\left(\frac{3}{2}g_{\alpha_2}+g_{\alpha_4}\right)\mathcal{U}\mathcal{T}'' = \mathcal{T}_0\left(1+8\rho^*\frac{\rho_0^*-8}{(\rho_0^*-4)^3}\right)+1-\mathcal{U} , \quad (23)$$

$$\frac{3}{2}\mathcal{T} - \frac{45}{16}g_\lambda \mathcal{T}^{1/2}\mathcal{T}' + \frac{9}{16}\left(\frac{2}{3}g_{\beta_1} - g_{\beta_2}\right)\mathcal{T}\mathcal{U}\mathcal{U}''$$
$$= \frac{3}{2}\mathcal{T}_0 + \frac{1}{2}(1-\mathcal{U})^2 + \mathcal{T}_0\left(1 + \frac{8\rho_0^*(\rho_0^*-8)}{(\rho_0^*-4)^3}\right)(1-\mathcal{U})\,. \tag{24}$$

In writing these equations use has been made of the relation $\mathcal{R}(s) = 1/\mathcal{U}(s)$. Notice that the functions g_i depend on s through the ratio $\rho_0^*/\mathcal{U}$. Further, Eqs. (23) and (24) involve the values of the density and temperature of the cold state. Following the work of Frezzotti and Sgarra [8], we will characterize the hydrodynamic profiles in terms of $M_B = 1/\sqrt{(5/3)\mathcal{T}_0}$ and $E = (3/\sqrt{2})\rho_0^*\chi_c(\rho_0^*)$. The parameter M_B represents a kind of upstream Mach number, while E is the ratio of the molecular diameter to the reference mean free path at the cold state. Fixing the value of E (which amounts to fixing the value of the density at the cold end) and the Mach number M_B (which specifies the value of the temperature at the cold end) and noting that the corresponding slopes at the cold end must be zero yields a well posed mathematical problem. Its solution, however, must be carried out numerically. Because the mathematical stability of the system of equations is directional [11], the numerical integration has to start at the hot equilibrium state. The conditions at this state follow from the Rankine-Hugoniot relations (4)–(6). We have used the adaptive procedure of a computer algebra system [12] to solve Eqs. (23) and (24) setting $\mathcal{U}(s_0) = \mathcal{U}_1 + 6\times10^{-6}$, $\mathcal{T}(s_0) = \mathcal{T}_1$, and choosing the initial integration point s_0 and the slopes $\mathcal{U}'(s_0)$ and $\mathcal{T}'(s_0)$ such as to minimize the difference between $\mathcal{U}(0)$ and a prescribed value that fixes the origin of the shock front, typically $(\mathcal{U}_0+\mathcal{U}_1)/2$.

A comparison of our results with those of Frezzotti and Sgarra [8] is displayed in Fig. 1, where we show the reduced density profiles for the case $E = 0$ and $M_B = 4$. In this figure we have also included the profiles predicted by the Navier-Stokes equations as well as those obtained through the use of Holian's conjecture [13], in which, in order to go beyond the Navier-Stokes level, the temperature dependence of the transport coefficients is through the (component of) temperature in the direction of shock wave propagation rather than the average temperature. A motivation for considering such a comparison lies on the fact that, on the one hand, it seems interesting to assess whether the value of M_B affects the trends already observed by Holian *et al.* [13], while on the other the kinetic equation considered in Ref. [8] is only compatible with the revised Enskog theory beyond the Navier-Stokes level for a dilute gas. As can be clearly seen, the Burnett equations improve the agreement with the simulation data as compared to the Navier-Stokes equations. Regarding the results using Holian's conjecture, the Burnett predictions are also superior in the hot region, seemingly capturing much better the relaxation mechanism. However, the performance on the cold side of the shock front is better if one uses the modified version of the Navier-Stokes theory. To close the discussion of the results for a low-density gas, i.e., $E = 0$, we must point out that the same qualitative trends are observed at high Mach numbers.

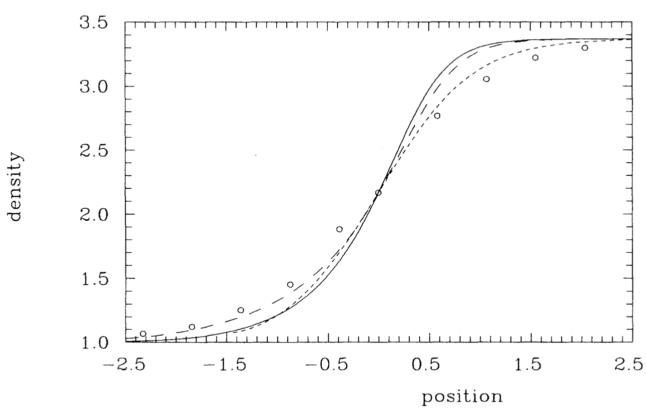

FIG. 1. Reduced density profiles $\mathcal{R}(s)$ vs position s for $E = 0$ and $M_B = 4$. We consider the results derived from the Navier-Stokes theory (—), from Holian's conjecture (- - -), and from the linearized Burnett theory (- - - -). Circles correspond to the simulation data taken from Ref. [8]. Note that the origin in this figure has been chosen to coincide with the one used in the simulation.

For the sake of analyzing the difference between the profiles predicted by the Navier-Stokes and Burnett theories at moderate density, it seems convenient to consider the limiting case of infinite Mach number. In this case, the gradients in the hydrodynamic variables are large so that the deviations from the linear laws (Navier-Stokes) can be relevant. Unfortunately, to our knowledge, no simulation results for strong shock waves in a dense hard-sphere gas are available. Therefore, in Figs. 2 and 3 we show, for the purposes of illustration only, the reduced velocity and temperature profiles for $E = 0.2$ and $E = 0.4$. The effect of the nonlinear laws is greater on the velocity profiles. Both theories lead to the expected result that the density jump across the shock is reduced as E increases. It appears that the Burnett theory predicts that as soon as the density is not zero, the symmetry of the

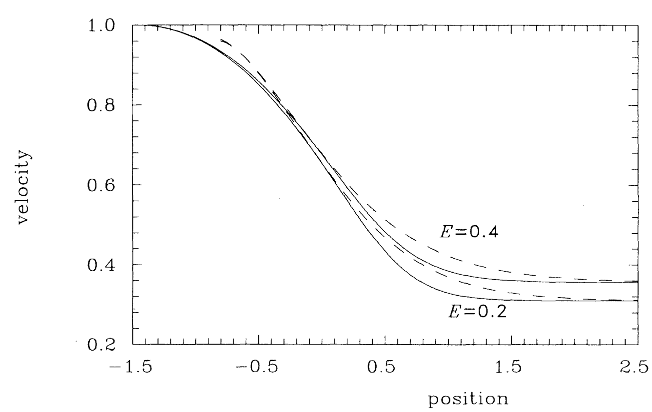

FIG. 2. Reduced velocity profiles $\mathcal{U}(s)$ for $M_B = \infty$ and two values of E. The solid lines correspond to the Navier-Stokes results while the dashed lines correspond to the linearized Burnett theory.

velocity profile observed for a dilute hard-sphere gas [13] is lost. Note, however, that the results on the cold side of the front far away from the origin are somewhat open to question since the numerical instabilities associated with the system of differential equations of this theory do not allow convergence of the solution.

In summary, in this paper we have examined the effect of using the linearized Burnett equations for the analysis of shock waves in a dense gas within the revised Enskog theory. While the comparison with the simulation results and other hydrodynamic approximations is clearcut only in the case of a low-density gas, where the Burnett equations are superior, we have also predicted profiles for moderate density and high Mach numbers. Our expectation is that these predictions stimulate the performance of simulations under these conditions. The very recent development of a modification of the direct simulation Monte Carlo method [14] certainly supports the likelihood of fulfilling such expectation.

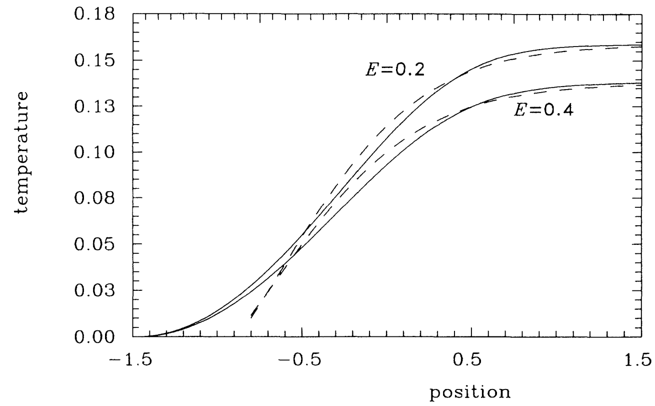

FIG. 3. Reduced temperature profiles $\mathcal{T}(s)$ for $M_B = \infty$ and two values of E. The solid lines correspond to the Navier-Stokes results while the dashed lines correspond to the linearized Burnett theory.

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