Simple and accurate theory for strong shock waves in a dense hard-sphere fluid

J. M. Montanero*
Departamento de Electrónica e Ingeniería Electromecánica, Universidad de Extremadura, E-06071 Badajoz, Spain

M. López de Haro†
Centro de Investigación en Energía, UNAM, Apartado Postal 34, Temixco, Morelos 62580, Mexico

A. Santos‡ and V. Garzó§
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

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Following an earlier work by Holian *et al.* [Phys. Rev. E **47**, R24 (1993)] for a dilute gas, we present a theory for strong shock waves in a hard-sphere fluid described by the Enskog equation. The idea is to use the Navier-Stokes hydrodynamic equations but taking the temperature in the direction of shock propagation rather than the actual temperature in the computation of the transport coefficients. In general, for finite densities, this theory agrees much better with Monte Carlo simulations than the Navier-Stokes and (linear) Burnett theories, in contrast to the well-known superiority of the Burnett theory for dilute gases. [S1063-651X(99)13212-4]

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The normal shock wave problem has been considered for a long time as the prototype to analyze far from equilibrium situations. Shock waves occupy a small and rapidly moving transition region in space that connects two different equilibrium states. One of them corresponds to a relatively cold low-pressure region and the other one to a relatively hot high-pressure region. Due to the abrupt spatial variations of the hydrodynamic fields, the search for accurate theories to fully describe such variations is still an ongoing task. Among the efforts carried out so far, continuum approaches have played an important role. They have been complemented by computer simulations, both using molecular dynamics [1,2] and the direct simulation Monte Carlo methods [3]. These simulations have been crucial in assessing the reliability and merits of the different continuum descriptions.

One of the difficulties associated with continuum approaches is the fact that in general the transport coefficients must be somewhat empirically adjusted. A possible way to overcome such limitation is to use the results stemming out of microscopic formulations. In the case of a dilute gas, the Chapman-Enskog expansion [4] of the Boltzmann equation provides explicit formulas for the transport coefficients both in the Navier-Stokes (first order in gradients) and Burnett (products of two gradients and second order in derivatives) approximations [4]. In these systems, Fiscko and Chapman [5] were the first to calculate hypersonic Burnett shock solutions up to Mach number $M=50$ and, by comparison with their own direct simulation Monte Carlo data, showed that the Burnett equations were more accurate than the Navier-Stokes (NS) equations for the description of normal shock structures. Later on, Salomons and Mareschal [2] confirmed such predictions in a pioneering paper using molecular dynamics for a Mach number $M=134$. Since nevertheless the NS equations provide a reasonable description and have a much simpler structure, Holian [6] introduced a slight modification to these equations to account for the fact that the component of temperature T_{xx} in the direction of shock propagation always exceeds the total average temperature T. The modification, designated as Holian's conjecture, consists of replacing T by T_{xx} in the NS transport coefficients and leads to a substantial improvement of the agreement with the molecular dynamics results over the standard NS equations [7]. An attempt to provide a kinetic foundation for Holian's conjecture has been recently reported by Uribe *et al.* [8]. In another paper [9], the same authors computed the velocity and temperature profiles for $M=134$ and gave further evidence that the Burnett theory is superior to both Holian's conjecture and the NS theory. The question arises as to whether the above conclusions may be extrapolated to dense fluids where new (potential) contributions to the transport coefficients are present. However, since the density dependence of the transport coefficients is not known in general, in order to provide an answer to the above question it is convenient to consider the hard-sphere model. For this model, the Enskog theory [10] gives a reliable description over the entire fluid domain. In the context of the Enskog equation, previous results [11] indicate that surprisingly the NS predictions are better than those of the (linear) Burnett theory at high Mach numbers. In view of these results and of the trend observed in the dilute gas once Holian's recipe was introduced, the natural next step is to test whether the above recipe, when properly extended, will yield the best overall performance. This is the main goal of this paper.

The component of the temperature in the direction of shock propagation, say x, is $T_{xx}=(m/\rho k_B)P_{xx}^k$, where m is the mass of a molecule, k_B is the Boltzmann constant, ρ is the mass density, and P_{xx}^k refers to the *kinetic* part of the xx normal component of the pressure tensor. This latter quantity can easily be identified from the fact that the pressure tensor

*Electronic address: jmm@unex.es
†Also at Programa de Simulación Molecular of the Instituto Mexicano del Petróleo. Electronic address: malopez@servidor.unam.mx
‡Electronic address: andres@unex.es
§Electronic address: vicenteg@unex.es

may be written as $\mathsf{P}=\mathsf{P}^k+\mathsf{P}^c$, with P^c indicating the collisional transfer contributions [4]. Holian's recipe consists of describing the shock wave by means of the NS equations but modifying the thermal dependence of the transport coefficients through the substitution of T by T_{xx}. In the NS approximation, the constitutive equations for a planar shock wave read $P_{xx}^k=(\rho k_B T/m)-\frac{4}{3}\mu^k u'$, $P_{xx}=p-(\frac{4}{3}\mu+\kappa)u'$, and $q_x=-\lambda T'$. Here, p is the hydrostatic pressure, u is the flow velocity, q_x is the heat flux, and u' and T' are the gradients of the velocity and temperature, respectively. In addition, $p=(\rho k_B T/m)[1+4\eta\chi(\eta)]$ with $\eta\equiv\pi\rho\sigma^3/6m$ being the packing fraction, σ the sphere diameter, and $\chi(\eta)$ the equilibrium pair correlation function at contact. The explicit expressions for the transport coefficients within the Enskog theory are [4]

$$\mu^k=\frac{1}{\chi(\eta)}[1+\tfrac{8}{5}\eta\chi(\eta)]\mu_B, \tag{1}$$

$$\kappa=\frac{4}{9}\left(\frac{\rho}{m}\right)^2\sigma^4\chi(\eta)(\pi m k_B T)^{1/2}, \tag{2}$$

$$\mu=\frac{1}{\chi(\eta)}[1+\tfrac{8}{5}\eta\chi(\eta)]^2\mu_B+\tfrac{3}{5}\kappa, \tag{3}$$

$$\lambda=\frac{1}{\chi(\eta)}[1+\tfrac{12}{5}\eta\chi(\eta)]^2\lambda_B+\frac{3}{2}\frac{k_B}{m}\kappa. \tag{4}$$

Here, μ_B and λ_B are the shear viscosity and the thermal conductivity of a dilute hard-sphere gas, respectively. Their values are [4]

$$\mu_B=1.0160\times\frac{5}{16}\left(\frac{m k_B T}{\pi}\right)^{1/2}\sigma^{-2}, \tag{5}$$

$$\lambda_B=1.0251\times\frac{15}{4}\frac{k_B}{m}\mu_B. \tag{6}$$

Note that all the Enskog transport coefficients are proportional to $\sqrt{T}$, i.e., $\{\mu(\rho,T),\kappa(\rho,T),\lambda(\rho,T)\}\equiv\{\tilde{\mu}(\rho),\tilde{\kappa}(\rho),\tilde{\lambda}(\rho)\}\sqrt{T}$. It still remains to specify T_{xx} in terms of the hydrodynamic fields ρ, u, and T. To do that we will consider two identities. First, we will take into account the Rankine-Hugoniot condition for the conservation of momentum [12], i.e., $P_{xx}(x)+\rho(x)u^2(x)=p_0+\rho_0 u_0^2=p_1+\rho_1 u_1^2$, where the subscript 0 refers to the unshocked cold equilibrium state ($x\to-\infty$, upstream) while the subscript 1 refers to the shocked hot equilibrium state ($x\to+\infty$, downstream). Secondly, according to the NS approximation, $(P_{xx}^k-\rho k_B T/m)/(P_{xx}-p)=\tilde{\mu}^k/(\tilde{\mu}+\frac{3}{4}\tilde{\kappa})\equiv A(\rho)$. From both identities, one gets

$$T_{xx}=T\{1-[1+4\eta\chi(\eta)]A(\rho)\}+A(\rho)u\left\{\frac{T_0}{u_0}[1+4\eta_0\chi(\eta_0)]+\frac{m}{k_B}(u_0-u)\right\}. \tag{7}$$

In writing Eq. (7) we have chosen the first equality of the Rankine-Hugoniot condition. It is easy to see that the expression for T_{xx} reduces to the one derived in Ref. [7] in the low-density limit. Replacing T by T_{xx} in the explicit expressions for the transport coefficients and subsequent substitution of the latter into the NS equations completes the generalization of Holian's recipe to the case of a dense hard-sphere fluid.

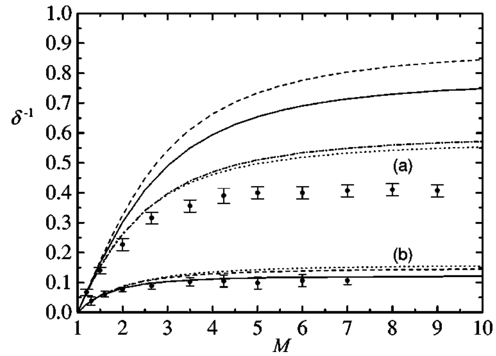

FIG. 1. Plot of the reciprocal shock thickness (in units of the mean free path ℓ_0) as a function of the Mach number M for (a) $\eta_0=0$ and (b) $\eta_0=0.2$ as obtained from the Holian theory (——), the Navier-Stokes theory (— — —), the linearized Burnett theory (- - - -), and the full Burnett theory (— - — -). The symbols are simulation results.

Now we are in a position to check the performance of the different continuum approaches by comparison with computer simulations. Here, we use the recently proposed Enskog simulation Monte Carlo (ESMC) method [13], which is an extension of the well-known direct simulation Monte Carlo (DSMC) method [3] to simulate the Boltzmann equation. The ESMC method has proven to be a valuable tool to numerically solve the Enskog equation. It is important to mention that while in the case of dilute gases one knows up to the complete (linear and nonlinear) Burnett transport coefficients, those of the Enskog equation have been determined explicitly only up to the linear Burnett order [14]. For the sake of the presentation of the results, we take the packing fraction η_0 and the Mach number $M=u_0/a_0$ as the relevant independent parameters of the problem. Here, a_0 is the upstream speed of sound whose expression [11] can be obtained from thermodynamic relations. As usual, the origin $x=0$ is chosen at the point where $u=(u_0+u_1)/2$. As for the pair correlation function at contact we take the Carnahan-Starling approximation [15], i.e., $\chi(\eta)=(1-\eta/2)/(1-\eta)^3$. In the context of the continuum description, the task is now to solve a set of nonlinear coupled differential equations for the hydrodynamic fields subjected to the Rankine-Hugoniot conditions [12]. The solution is carried out numerically and the details of the method have been described in Ref. [16].

Since the velocity and temperature profiles exhibit in this problem a high degree of symmetry, perhaps a better candidate to assess the merits of the different theories is the shock thickness, whose reciprocal is defined as the maximum value of the normalized density gradient [3], i.e., $\delta^{-1}=(\rho_1-\rho_0)^{-1}(d\rho/dx)_{\max}$. In Fig. 1 we display the Mach number dependence of δ^{-1} for two values of the packing fraction η_0 in the upstream region. The shock thickness is measured in units of the mean free path at the cold region, $\ell_0=[\sqrt{2}\pi\rho_0\chi(\eta_0)\sigma^2/m]^{-1}$. The error bars on the simulation points indicate the uncertainty associated with statistical

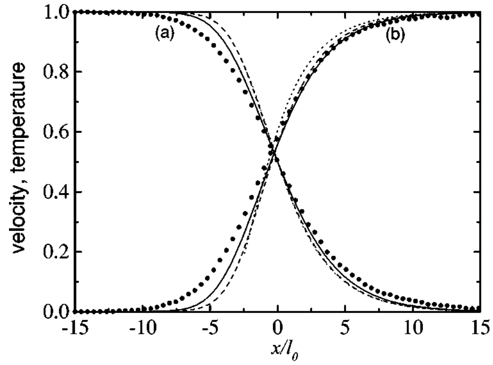

FIG. 2. Profiles of (a) the reduced velocity $(u-u_1)/(u_0-u_1)$ and (b) the reduced temperature $(T-T_0)/(T_1-T_0)$ for $\eta_0=0.2$ and $M=3.5$. The solid line refers to the Holian theory, the dashed line to the Navier-Stokes theory, and the dotted line corresponds to the (linear) Burnett theory. The symbols are simulation results.

fluctuations and with the location of $(d\rho/dx)_{\max}$. In general, we see that all the theoretical predictions underestimate the shock thickness δ. In the low-density regime ($\eta_0=0$), it is clear that the Burnett theory leads to a better agreement with simulations than both the NS and Holian's predictions. A similar conclusion was also reached in Ref. [8]. However, it is interesting to notice that the best overall performance is given by the *linearized* rather than the *full* (linear plus nonlinear) Burnett equations. In fact, for $\eta_0=0$ and $M=134$ (which is the case studied in Refs. [2], [7], and [8]), we get $\delta^{\rm NS}=1.13\ell_0$ for the NS theory, $\delta^{\rm H}=1.27\ell_0$ for the Holian theory, $\delta^{\rm B}=1.68\ell_0$ for the full Burnett theory, and $\delta^{\rm LB}=1.74\ell_0$ for the linear Burnett theory, while the thickness estimated from the molecular dynamics results of Ref. [2] is $\delta=2.3\ell_0$. This casts doubts on the likelihood that one should retain super-Burnett and higher order gradient terms to get a better description as the Mach number is increased. In passing we note that in view of the trend observed in Fig. 1, the molecular dynamics result for the shock thickness at $M=134$ is compatible with the ones derived with the ESMC method for smaller values of the Mach number. For a finite density (exemplified by the case $\eta_0=0.2$), the present results confirm our earlier finding [11] that the NS predictions are surprisingly superior to the (linear) Burnett predictions for high Mach numbers (say, for instance $M\approx3$). In this case we have enlarged the range of values of M in the simulations up to $M=7$. Moreover, the NS predictions are *clearly* improved when Holian's recipe is introduced, as indicated by the fact that, when the error bars are accounted for, all the simulation results fall on top of the theoretical Holian line. Thus for $M=3.5$ and $\eta_0=0.2$, one gets for the shock-wave thickness $\delta^{\rm NS}=8.09\ell_0$, $\delta^{\rm LB}=7.76\ell_0$, $\delta^{\rm H}=9.27\ell_0$ while the simulation result obtained from the ESMC method is $\delta=(10\pm1)\ell_0$. It is worthwhile noting that, in general, the hydrodynamic theories tend to provide a better description of the shock-wave structure as the density increases. This can be partially explained by the fact that the thickness, when expressed in units of the mean free path, increases with the density.

As a further illustration of the superiority of using Holian's recipe, in Figs. 2 and 3 we show the (reduced) velocity and temperature, the stress $P_{xx}-p$, and the heat flux q_x profiles, for $M=3.5$ and $\eta_0=0.2$. Due to numerical instabilities,

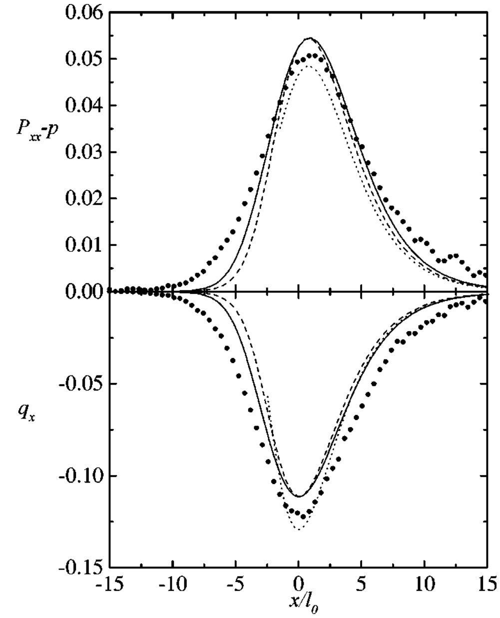

FIG. 3. The same as in Fig. 2, but for the stress $P_{xx}-p$, measured in units of $2k_BT_0/\ell_0^3$, and for the heat flux q_x, measured in units of $m(2k_BT_0/m)^{3/2}/\ell_0^3$.

the linear Burnett profiles are interrupted on the cold side [16]. It must be pointed out that although the theoretical curves fail to capture the longer relaxation towards the cold end equilibrium values reflected in the simulation results, in the case of the velocity and temperature profiles the hot region is rather well described by the Holian theory. The agreement is not so good for the momentum and heat fluxes, but nevertheless the behavior with respect to the shock thickness is again manifested in an improvement of the Holian theory over the remaining continuum approaches.

In summary, in this paper we have generalized Holian's recipe to describe planar shock waves in a dense hard-sphere fluid within the Enskog theory. The comparison with simulation results allows us to assess the merits of several continuum approaches, including also the dilute regime as a particular case. From a practical point of view and taking into account the data we have computed for a range of densities and Mach numbers, we can conclude that for $M\gtrsim1.5$, only if $\eta_0\lesssim0.1$, the (linear) Burnett theory provides the best description. Outside this density range, the Holian theory is clearly superior to all other continuum approaches. A further asset of this theory is that it combines reasonable accuracy for such a complicated problem with relative simplicity, since it only takes into account the *linear* relationships between fluxes and gradients. The only new ingredient is the use of the temperature in the direction of shock propagation rather than the average temperature in the linear transport coefficients. Note that, although the Holian constitutive equations are *formally linear*, they incorporate *nonlinear* effects through the dependence of the transport coefficients on the momentum flux. This naturally leads to a non-Newtonian description where the viscosities and the thermal conductivity depend in a nonlinear way on the strain rate $u'(x)$. Therefore, instead of the inclusion of additional higher order gradient expansions that would greatly complicate the actual solution and may be flawed by the asymptotic character of the Chapman-Enskog expansion, we favor the alternative strategy of using *linear laws* with an adequate thermal dependence of the transport coefficients. As a final point, one would hope that the same kind of recipe would work not only for dense hard-sphere gases although for other fluids the extension is not clearcut. In this connection, the performance of more simulations would be welcome to decide whether the above expectation is fulfilled.

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