

The Structure of an Infinitely Strong Shock Wave for Hard Sphere Molecules

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Abstract. The structure of an infinitely strong shock wave (i.e., a shock wave with infinitely large upstream Mach number) is investigated on the basis of the Boltzmann equation. The velocity distribution function is expressed as a sum of a multiple of the Dirac delta function, centered at the upstream bulk velocity, and a remainder. Strong evidence that the remainder has a singularity in the molecular velocity space was provided by a previous Monte Carlo simulation for a hard-sphere gas [Cercignani *et al.*, Phys. Fluids **11**, 2757 (1999)]. Then, the singularity was confirmed and clarified with sufficient accuracy by a precise numerical analysis by means of a finite-difference method. More specifically, the equation for the remainder, which contains the linear collision term linearized around the delta function and the nonlinear collision term, is solved numerically for a hard-sphere gas after the nonlinear collision term is replaced by the BGK collision model. The present paper reports on the main result of this analysis.

INTRODUCTION

H. Grad [1] suggested that the limit of the shock profile for the upstream Mach number going to infinity exists (at least for collision operators with a finite collision frequency) and is given by a multiple of the delta function, centered at the upstream bulk velocity, plus a comparatively smooth function, i.e., the velocity distribution function f can be decomposed as $f = \rho_\delta \delta(\boldsymbol{\xi} - \mathbf{u}_\infty) + \tilde{f}$, where δ is the Dirac delta function, $\boldsymbol{\xi}$ is the molecular velocity, and $\mathbf{u}_\infty$ is the flow velocity at upstream infinity. The equation for the remainder $\tilde{f}$, which is not hard to derive, seems to be more complicated than the Boltzmann equation itself, but the presumed smoothness of its solution should allow a simple approximate solution to be obtained. Grad investigated the simplest choice for the smooth remainder, a Maxwellian distribution, the parameters of which are determined by the conservation equations. Recently the problem was revisited by Cercignani *et al.* [2], who provided a survey on the shock wave problem with particular attention to an infinitely strong shock and showed that a Monte Carlo simulation for a hard sphere gas provides strong evidence for a singularity of the remainder $\tilde{f}$ in velocity space. The singularity appears to be given by $|\boldsymbol{\xi} - \mathbf{u}_\infty|^{-1}$.

This singularity was the object of a further investigation by a deterministic, more accurate method presented by Takata *et al.* [3]. They obtained a deterministic (rather than Monte Carlo) numerical solution for a hard-sphere gas, which confirms the previous results with considerable accuracy. The method used in their paper is based on the idea that the singularity is essentially determined by the Boltzmann collision operator L_δ linearized about the delta function, first introduced by Grad [1] and studied by Cafisch [4]. That is, Takata *et al.* replaced the nonlinear collision term for the remainder $\tilde{f}$ by a BGK collision model [5,6], keeping the hard-sphere interaction in L_δ . This replacement, which simplifies the numerical procedure dramatically, enabled them to perform an accurate numerical analysis.

The interest of the problem lies in the fact that, as conjectured by Cercignani *et al.* [2], the aforementioned singularity depends on the molecular model. If the remainder $\tilde{f}$ multiplied by the molecular velocity component $\xi_\perp$ perpendicular to the direction of gas flow is integrated over the full range of the component, and if the result is plotted as a function of the component $\xi_\parallel$ parallel to the flow, the singularity manifests itself as a

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corner point at the upstream bulk velocity $\mathbf{u}_-$. The angle at the corner point would change depending on the molecular model. This suggests that information on the intermolecular potential might be obtained from the measurement of the (integrated) velocity distribution. For this reason, we have started the research project to clarify the structure of the singularity for various molecular models and obtained the result for hard-sphere molecules. In the present paper, as the first report of the project, we summarize the result for hard-sphere molecules, giving a formulation for more general molecular models.

BASIC EQUATION

We consider a steady flow of a gas through a standing normal shock wave and investigate the structure of the shock wave in the extreme case of infinitely large upstream Mach number on the basis of the Boltzmann equation. In this case, the upstream Maxwellian reduces to $\rho_- \delta(\boldsymbol{\xi} - \mathbf{u}_-)$, where ρ_- is the density of the gas at upstream infinity. To analyze this problem, we first decompose the velocity distribution function f as mentioned in Introduction, i.e.,

$$f = \rho_\delta(X_1) \delta(\boldsymbol{\xi} - u_- \mathbf{i}) + \tilde{f}, \quad (1)$$

where the X_1 axis of the space coordinates X_i is taken in the direction of the gas flow, ρ_δ is a function of X_1 , and $\mathbf{i}$ is the unit vector in the X_1 direction (therefore, $\mathbf{u}_- = u_- \mathbf{i}$). Then the Boltzmann equation leads to the following equations for $\tilde{f}$ and ρ_δ :

$$\xi_1 \frac{\partial \tilde{f}}{\partial X_1} = L_\delta(\tilde{f}) + Q(\tilde{f}, \tilde{f}), \quad u_- \frac{d\rho_\delta}{dX_1} = -[\nu(\tilde{f})]_{\boldsymbol{\xi}=u_- \mathbf{i}} \rho_\delta, \quad (2)$$

where

$$L_\delta(\tilde{f}) = \rho_\delta [2Q_+(\delta(\boldsymbol{\xi} - u_- \mathbf{i}), \tilde{f}) - \nu(\delta(\boldsymbol{\xi} - u_- \mathbf{i})) \tilde{f}], \quad (3)$$

$$Q(g, h) = Q_+(g, h) - \frac{1}{2} [\nu(g)h + \nu(h)g], \quad (4)$$

$$Q_+(g, h) = \frac{1}{2m} \int [g(\boldsymbol{\xi}'_*)h(\boldsymbol{\xi}') + g(\boldsymbol{\xi}')h(\boldsymbol{\xi}'_*)] B(\theta, |\mathbf{V}|) d\theta d\psi d\boldsymbol{\xi}_*, \quad (5)$$

$$\nu(g) = \frac{1}{m} \int g(\boldsymbol{\xi}_*) B(\theta, |\mathbf{V}|) d\theta d\psi d\boldsymbol{\xi}_*, \quad (6)$$

$$\boldsymbol{\xi}'_* = \boldsymbol{\xi}_* - (\mathbf{V} \cdot \boldsymbol{\alpha}) \boldsymbol{\alpha}, \quad \boldsymbol{\xi}' = \boldsymbol{\xi} + (\mathbf{V} \cdot \boldsymbol{\alpha}) \boldsymbol{\alpha}, \quad \mathbf{V} = \boldsymbol{\xi}_* - \boldsymbol{\xi}. \quad (7)$$

Here, m is the mass of a molecule, $\boldsymbol{\alpha}$ is a unit vector, $B(\theta, |\mathbf{V}|)$ is a nonnegative function depending on the intermolecular potential, θ and ψ are, respectively, the polar and the azimuthal angle of $\boldsymbol{\alpha}$ expressed by the polar coordinates with the polar axis in the direction of $\mathbf{V}$, and the domain of integration in Eqs. (5) and (6) is $0 \leq \theta \leq \pi/2$, $0 \leq \psi < 2\pi$, and the whole space of $\boldsymbol{\xi}_*$. For hard-sphere molecules $B = \sigma^2 |\mathbf{V}| \sin \theta \cos \theta$ with σ being the diameter of a molecule, and for the Maxwellian molecules $B = \beta(\theta)$ with $\beta(\theta)$ being a function of θ only. The boundary conditions are as follows:

$$\tilde{f} \rightarrow 0, \quad \rho_\delta \rightarrow \rho_-, \quad \text{when } X_1 \rightarrow -\infty, \quad (8a)$$

$$\tilde{f} \rightarrow f_{M+} = \frac{\rho_+}{(2\pi RT_+)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - u_+ \mathbf{i}|^2}{2RT_+}\right), \quad \text{when } X_1 \rightarrow \infty, \quad (8b)$$

where R is the gas constant per unit mass, and ρ_+ , T_+ , and $u_+ \mathbf{i}$ are, respectively, the density, temperature, and flow velocity at downstream infinity, which are related to the upstream density ρ_- and flow velocity u_- by the Rankine-Hugoniot relations

$$\rho_+/\rho_- = u_-/u_+ = 4, \quad RT_+/u_-^2 = 3/16. \quad (9)$$

SOME TRANSFORMATIONS

In the present problem, we can seek the solution with cylindrical symmetry in the molecular velocity space, i.e., in the following form:

$$\tilde{f} = \tilde{f}(X_1, \xi_1, \eta), \quad \eta = (\xi_2^2 + \xi_3^2)^{1/2}. \quad (10)$$

The explicit expression of the linearized collision operator $L_\delta(\tilde{f})$ in this case was obtained by Caflisch [4]. That is, the $Q_+(\delta(\xi - u_- \mathbf{i}), \tilde{f})$ in $L_\delta(\tilde{f})$ can be expressed as

$$\begin{aligned} Q_+(\delta(\xi - u_- \mathbf{i}), \tilde{f}) = & 2 \int_{-\infty}^{\infty} \int_0^{\infty} \frac{H(A_1)H(A_2)}{\sqrt{A_1 A_2}} \\ & \times \frac{R_B(|\xi - u_- \mathbf{i}|, \sqrt{|\xi_* - u_- \mathbf{i}|^2 - |\xi - u_- \mathbf{i}|^2})}{|\xi - u_- \mathbf{i}|} \tilde{f}(X_1, \xi_{1*}, \eta_*) \eta_* d\eta_* d\xi_{1*}, \end{aligned} \quad (11)$$

where

$$A_1 = \eta\eta_* - |\xi - u_- \mathbf{i}|^2 + (\xi_1 - u_-)(\xi_{1*} - u_-), \quad A_1 = \eta\eta_* + |\xi - u_- \mathbf{i}|^2 - (\xi_1 - u_-)(\xi_{1*} - u_-), \quad (12a)$$

$$\xi_* = (\xi_{1*}, \xi_{2*}, \xi_{3*}), \quad \eta_* = (\xi_{2*}^2 + \xi_{3*}^2)^{1/2}, \quad (12b)$$

and $R_B(v, w)$ is defined in terms of B as

$$R_B(|\mathbf{V}| \cos \theta, |\mathbf{V}| \sin \theta) = \frac{1}{2m} \frac{1}{\sin \theta} [B(\theta, |\mathbf{V}|) + B(\pi/2 - \theta, |\mathbf{V}|)]. \quad (13)$$

Therefore, $R_B(v, w) = v$ for hard-sphere molecules. On the other hand, $\nu(\delta(\xi - u_- \mathbf{i}))$ in Eq. (3) and $[\nu(\tilde{f})]_{\xi=u_- \mathbf{i}}$ in Eq. (2) are expressed as

$$\nu(\delta(\xi - u_- \mathbf{i})) = \frac{2\pi}{m} \int_0^{\pi/2} B(\theta, |\xi - u_- \mathbf{i}|) d\theta, \quad (14)$$

$$[\nu(\tilde{f})]_{\xi=u_- \mathbf{i}} = \frac{4\pi^2}{m} \int_{-\infty}^{\infty} \int_0^{\infty} \int_0^{\pi/2} \tilde{f}(X_1, \xi_{1*}, \eta_*) B(\theta, |\xi_* - u_- \mathbf{i}|) \eta_* d\theta d\eta_* d\xi_{1*}. \quad (15)$$

As mentioned in Introduction, it is likely that the singularity occurring in $\tilde{f}$ is essentially determined by the linearized collision term $L_\delta(\tilde{f})$. In fact, we have checked that the linearized problem, obtained by dropping the nonlinear term $Q(\tilde{f}, \tilde{f})$ in Eq. (2), has a numerical solution which is qualitatively satisfactory (in particular, it exhibits the expected singularity) but fails to reach a Maxwellian downstream for particles traveling downstream (for particles traveling upstream this property is part of the boundary conditions). To simplify the numerical procedure, therefore, Takata *et al.* [3] replaced the nonlinear term by a BGK collision model [5,6] with a suitably adjusted collision frequency, keeping the hard-sphere interaction in L_δ . In fact, the main role of the quadratic collision term $Q(\tilde{f}, \tilde{f})$ is perceived to be that of obliging $\tilde{f}$ to go to a Maxwellian distribution in the entire velocity space. The replacement mentioned above is as follows:

$$Q(\tilde{f}, \tilde{f}) = A_c \tilde{\rho}(\tilde{f}_e - \tilde{f}), \quad (16)$$

where

$$\tilde{f}_e = \frac{\tilde{\rho}}{(2\pi R\tilde{T})^{3/2}} \exp\left(-\frac{|\xi - u_- \mathbf{i}|^2}{2R\tilde{T}}\right), \quad (17a)$$

$$\begin{aligned} \tilde{\rho} &= 2\pi \int_{-\infty}^{\infty} \int_0^{\infty} \tilde{f}(X_1, \xi_1, \eta) \eta d\eta d\xi_1, \quad \tilde{u} = \frac{2\pi}{\tilde{\rho}} \int_{-\infty}^{\infty} \int_0^{\infty} \xi_1 \tilde{f}(X_1, \xi_1, \eta) \eta d\eta d\xi_1, \\ \tilde{T} &= \frac{2\pi}{3R\tilde{\rho}} \int_{-\infty}^{\infty} \int_0^{\infty} |\xi - u_- \mathbf{i}|^2 \tilde{f}(X_1, \xi_1, \eta) \eta d\eta d\xi_1. \end{aligned} \quad (17b)$$

Here, A_c is a constant chosen in such a way that $A_c \rho_+$ is the mean collision frequency of the molecules in the equilibrium state at rest with density ρ_+ and temperature T_+ [$A_c = 4\sqrt{\pi R T_+}(\sigma^2/m)$ for hard-sphere molecules].

RESULT OF NUMERICAL ANALYSIS

The boundary-value problem to be solved consists of Eqs. (2) and (3), with the expressions (11), (14), and (15) and with the replacement (16), and the boundary conditions (8a) and (8b). It was analyzed numerically for hard-sphere molecules by means of an accurate finite-difference method in [3]. We summarize the result in the following subsections, where the origin $X_1 = 0$ is set at the point at which the density is equal to the mean of the upstream and downstream densities $[\rho = (\rho_- + \rho_+)/2]$.

Macroscopic quantities

We first show the results for the macroscopic quantities. The profiles of the density ρ , the flow velocity in the X_1 direction u , and the temperature T are shown in Fig. 1, where ρ_* , u_* , and T_* are the dimensionless quantities defined by

$$\rho_* = \frac{\rho - \rho_-}{\rho_+ - \rho_-}, \quad u_* = \frac{u - u_+}{u_- - u_+}, \quad T_* = \frac{T}{T_+}, \quad (18)$$

and l_- is the mean free path of the gas molecules in the equilibrium state at rest with density ρ_- , i.e., $l_- = (\sqrt{2}\pi\sigma^2\rho_-/m)^{-1}$. The figure also contains the profiles of the density ρ_δ of the delta-function part, the parallel temperature $T_\parallel$, and the perpendicular temperature $T_\perp$ [$T = (T_\parallel + 2T_\perp)/3$; see Eq. (20) below]. More precisely, $\rho_{\delta*}$, $T_{\parallel*}$, and $T_{\perp*}$ in Fig. 1 are the following dimensionless quantities

$$\rho_{\delta*} = \frac{\rho_\delta}{\rho_-}, \quad T_{\parallel*} = \frac{T_\parallel}{T_+}, \quad T_{\perp*} = \frac{T_\perp}{T_+}, \quad (19)$$

$T_\parallel$ and $T_\perp$ being defined by

$$T_\parallel = \frac{1}{R\rho} \int (\xi_1 - u)^2 f d\xi, \quad T_\perp = \frac{1}{2R\rho} \int (\xi_2^2 + \xi_3^2) f d\xi. \quad (20)$$

Figure 2 shows the comparison of the profiles of ρ , u , and T with those obtained by the Monte Carlo simulation in [2]. The transition shown in Fig. 1 is monotonic with respect to X_1 for ρ , u , and ρ_δ , whereas that for T , which is the sum of monotonic $2T_\perp/3$ and highly nonmonotonic $T_\parallel/3$, exhibits a very slight overshoot (0.28% of T_+). This overshoot is smaller than that observed in the Monte Carlo simulation (1% of T_+). The overshoot of almost the same magnitude was obtained for several different lattice systems as well as for some different choices of A_c in the BGK model. However, we cannot claim the presence of the overshoot definitely because

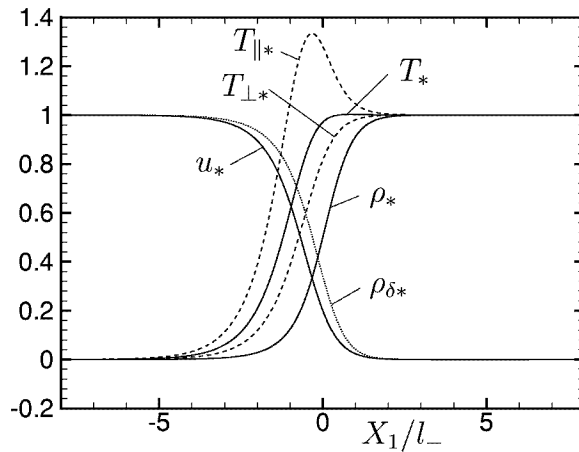


FIGURE 1. The profiles of the macroscopic quantities in the shock wave. The ρ_* , u_* , and T_* are defined by Eq. (18), while $\rho_{\delta*}$, $T_{\parallel*}$, and $T_{\perp*}$ are defined by Eq. (19).

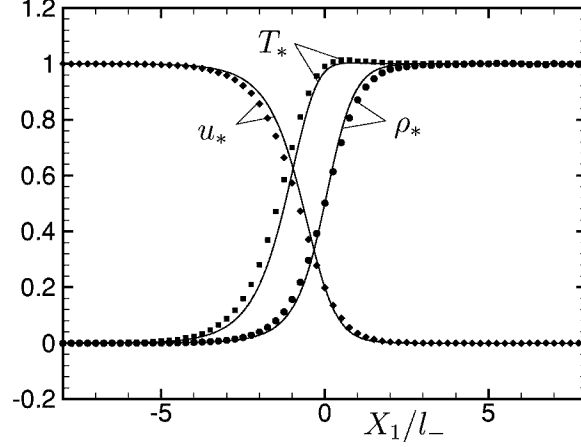


FIGURE 2. Comparison of the profiles of the density, flow velocity, and temperature with those by the DSMC computation. The ρ_* , u_* , and T_* are defined by Eq. (18). The solid lines indicate the deterministic numerical result [3], while the symbols $\bullet$, $\blacklozenge$, and $\blacksquare$ indicate the DSMC result [2].

its magnitude is close to the estimated error in the computation. Because of the use of the BGK model for the nonlinear collision term, the present result should not be expected to give the precise profiles for a hard-sphere gas. Nevertheless, it shows reasonable agreement with the result of Monte Carlo simulation.

Velocity distribution function

We next show the behavior of the non-delta-function part $\tilde{f}$ of the velocity distribution function. The contour lines $(u_-^2/\rho_-)\eta\tilde{f} = \text{const}$ at various points in the shock layer are plotted in the plane of ξ_1/u_- and η/u_- in Fig. 3, where the corresponding contour lines of the downstream Maxwellian f_{M+} are also shown by dashed lines. The figure exhibits the concentration of the contour lines at the point corresponding to the upstream bulk velocity $\xi_1 = u_-$, $\eta = 0$. The concentration of the contour lines means that the limiting value of $\eta\tilde{f}$ at $\xi_1 = u_-$, $\eta = 0$ is a function of the angle $\theta_\xi = \arctan(\eta/(\xi_1 - u_-))$ ($0 \leq \theta_\xi \leq \pi$), i.e.,

$$\lim_{\xi_1 \rightarrow u_-, \eta \rightarrow 0} \eta \tilde{f}(X_1, \xi_1, \eta) = F(X_1, \theta_\xi). \quad (21)$$

The numerical result of $F(X_1, \theta_\xi)/F_{\max}(X_1)$ at several points in the shock layer is shown as a function of θ_ξ by solid lines in Fig. 4(a), where $F_{\max}(X_1) = \max_{0 \leq \theta_\xi \leq \pi} F(X_1, \theta_\xi)$ and is given in Fig. 4(b). The fact that $F(X_1, \theta_\xi)$ turns out to be finite for any θ_ξ proves that $\tilde{f}$ diverges as $|\xi - u_- \mathbf{i}|^{-1}$. The fact that the θ_ξ dependence is not given by a constant times $\sin \theta_\xi$ [as seen from Fig. 4(a)] shows that the dependence on the Cartesian components of the molecular velocity exhibits a more complex singularity than a simple product of $|\xi - u_- \mathbf{i}|^{-1}$ by a regular function of these components. The concentration of the contour lines has been predicted by the Monte Carlo simulation in [2]. It was confirmed in a clearer way by the present deterministic computation.

Another aspect of the singularity can be viewed if one considers the following marginal velocity distribution function associated with $\tilde{f}$:

$$\tilde{h}(X_1, \xi_1) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(X_1, \xi) d\xi_2 d\xi_3 = 2\pi \int_0^\infty \eta \tilde{f}(X_1, \xi_1, \eta) d\eta. \quad (22)$$

The $(u_-/\rho_-)\tilde{h}$ versus ξ_1/u_- at various points in the gas is shown in Fig. 5. The singularity discussed above manifests itself as a corner point at $\xi_1 = u_-$. The angle of the corner depends on the position. It is relatively small at $X_1/l_- = -1$ and -0.6 and increases as the position moves downstream. The corner becomes invisible and $\tilde{h}$ approaches the corresponding marginal distribution of f_{M+} as X_1/l_- becomes large ($X_1/l_- = 1.4 \rightarrow 5$). The presence of the corner point at $\xi_1 = u_-$ was also anticipated by the Monte Carlo simulation (see Fig. 2 of [2]). But because of the noise or fluctuation intrinsic in the Monte Carlo simulation, it was not possible

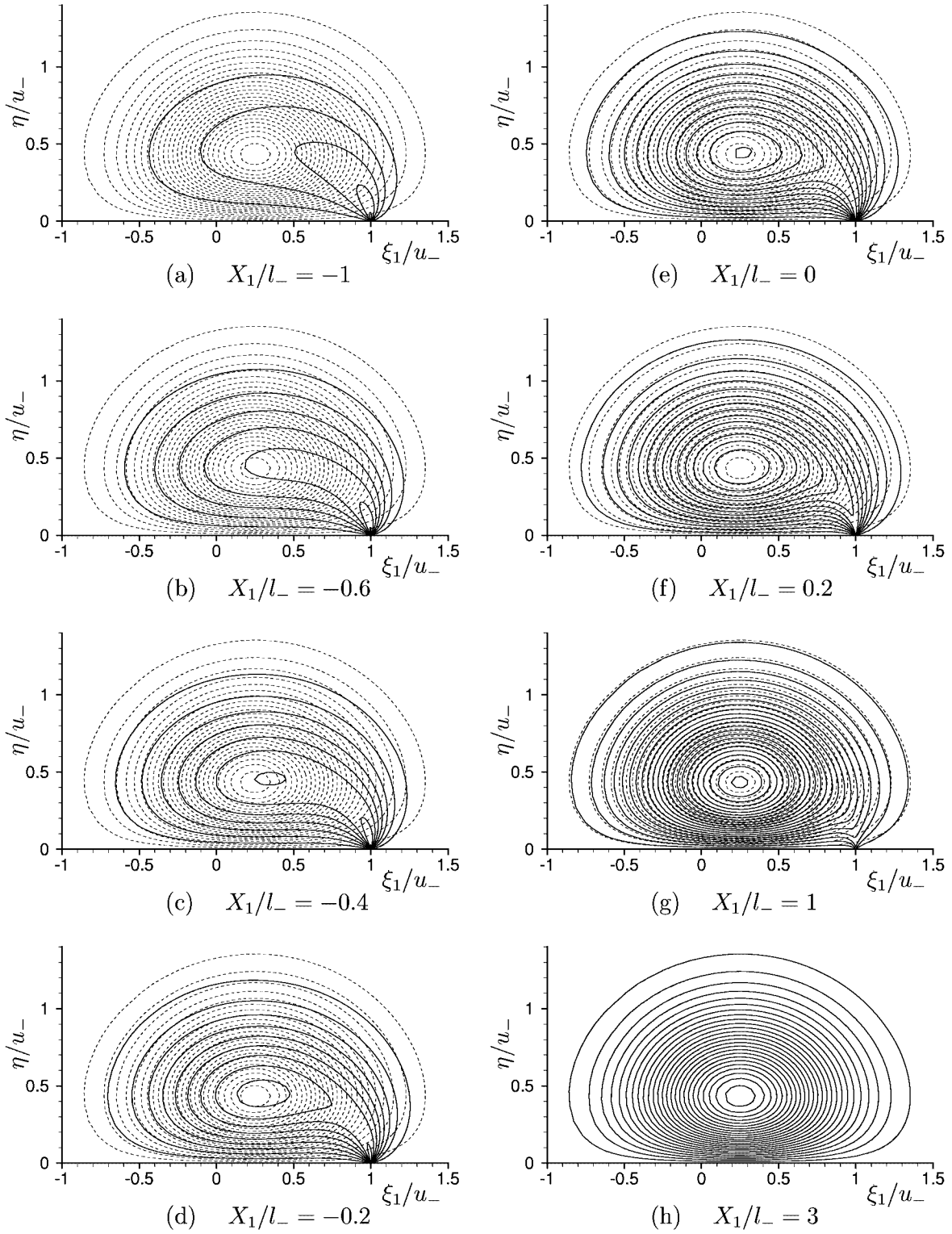


FIGURE 3. The contour lines $(u_-^2/\rho_-)\eta\tilde{f}(X_1, \xi_1, \eta) = \text{const}$ in the $\xi_1\eta$ -plane for various positions in the gas. (a) $X_1/l_- = -1$, (b) $X_1/l_- = -0.6$, (c) $X_1/l_- = -0.4$, (d) $X_1/l_- = -0.2$, (e) $X_1/l_- = 0$, (f) $X_1/l_- = 0.2$, (g) $X_1/l_- = 1$, (h) $X_1/l_- = 3$. Here, the dashed lines indicate the contour lines corresponding to the downstream Maxwellian distribution f_{M+} . The contour lines $(u_-^2/\rho_-)\eta\tilde{f} = 0.032m$ ($m = 1, 2, \dots$) are plotted (up to $m = 25$ for the Maxwellian). The outermost line corresponds to $m = 1$ for both distributions.

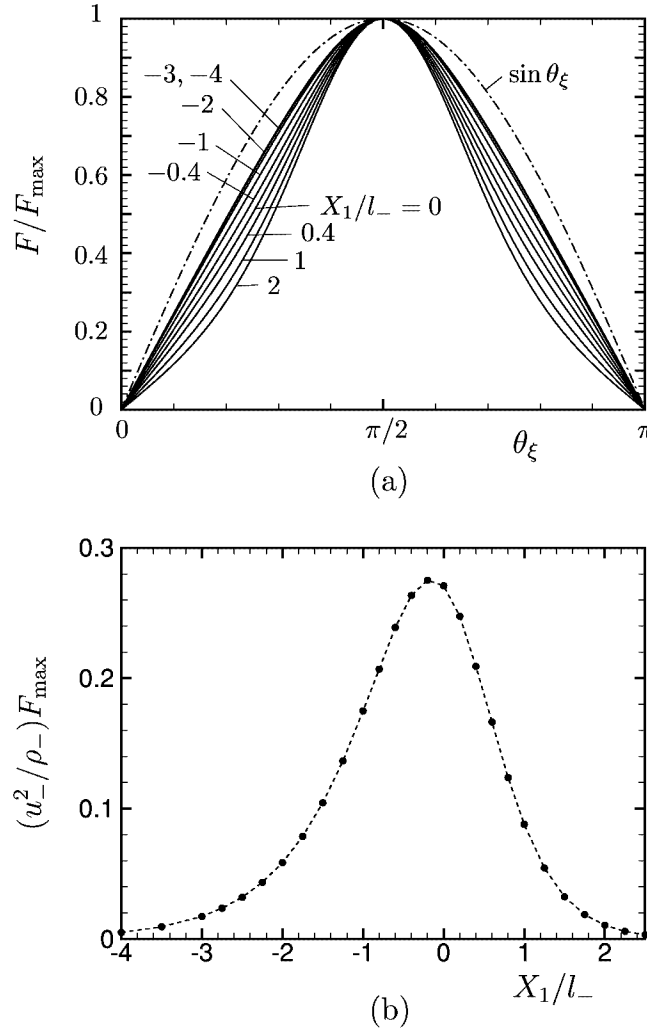


FIGURE 4. The functions $F(X_1, \theta_\xi)$ and $F_{\max}(X_1)$. (a) $F/F_{\max}$ for $X_1/l_- = -4, -3, -2, -1, -0.4, 0, 0.4, 1$ and 2 , (b) $F_{\max}$. Here, $F_{\max}(X_1) = \max_{0 \leq \theta_\xi \leq \pi} F(X_1, \theta_\xi)$. In (a), the solid line indicates the numerical result of $F/F_{\max}$, and the dot-dash line indicates $\sin \theta_\xi$.

to draw a definite conclusion. The present computation not only confirms the existence of the corner point clearly, but also gives detailed information about the corner angle.

CONCLUDING REMARKS

We have presented the results of numerical analysis [3] of the structure of an infinitely strong shock wave in a hard-sphere gas. We first split the velocity distribution function into a multiple of the delta function (delta part) and the remainder (non-delta part) and solved the equation for the latter (coupled with the density of the delta part) numerically by a finite-difference method. In the process of analysis, though the exact form of the linear collision term for the interaction between the delta and the non-delta part was retained, the nonlinear collision term for the non-delta part was replaced by the BGK collision model. The result confirms, in a clearer form, the singular behavior of the non-delta part found by a Monte Carlo simulation in a previous paper [2]. The information summarized in the present paper would give an insight required for a mathematically rigorous analysis of the singularity.

As mentioned in Introduction, the behavior of the singularity for different molecular models would give

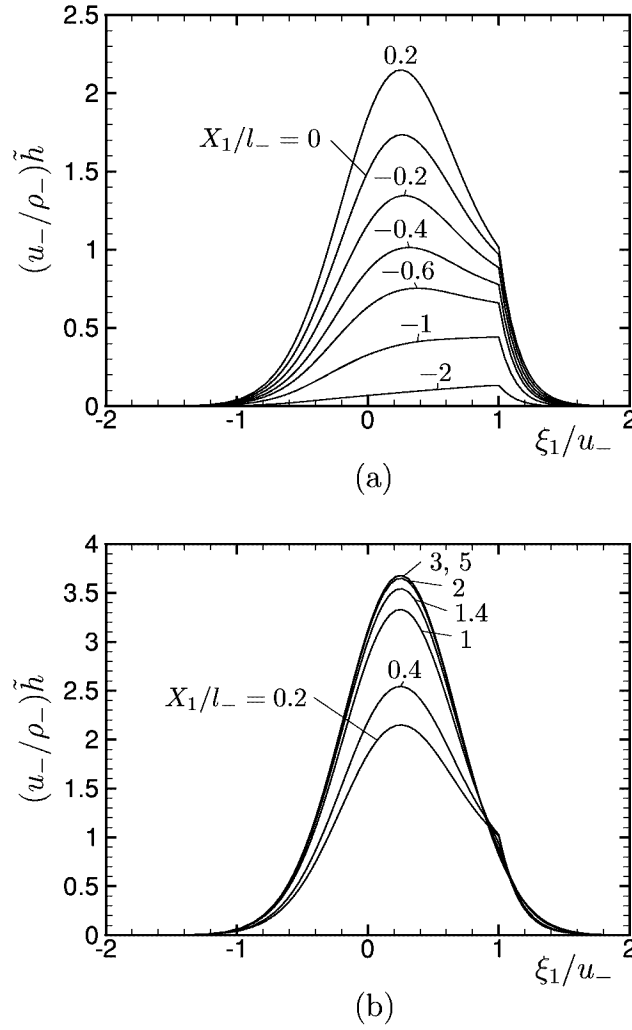


FIGURE 5. The marginal velocity distribution function $\tilde{h}(X_1, \xi_1)$ defined by Eq. (22) as a function of ξ_1 for various positions in the gas. (a) $-2 \leq X_1 / l_- \leq 0.2$, (b) $0.2 \leq X_1 / l_- \leq 5$.

information of physical interest and importance (see also the discussion at the end of [2]). Since the use of the BGK model for the nonlinear collision term for the non-delta part turned out to be successful, the extension of the analysis to molecular models other than hard spheres, such as the Maxwellian molecules, is not difficult. This will be the object of our future study.

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