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Kyoto University
STRUCTURE OF NORMAL SHOCK WAVES

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Abstract

The structure of normal shock waves is investigated numerically on the basis of the standard Boltzmann equation for hard-sphere molecules. The velocity distribution function as well as the macroscopic quantities are obtained accurately by a finite difference method where the collision term is computed directly without using the Monte-Carlo technique. The results are compared with the analytical solution for weak shock, Mott-Smith solution, and direct simulation Monte-Carlo result.

I. Introduction

The structure of normal shock waves is one of the most fundamental problems of the nonlinear Boltzmann equation. This problem has also been used by various authors as a test case of several methods and models (e.g. Refs. 1-10) and the standard solution based on the full Boltzmann equation gives useful information in the quantitative validation of them. Recently, a numerical method of the Boltzmann equation for hard-sphere molecules has been proposed and the accurate solution has been obtained.\textsuperscript{11} In the present paper, the numerical method is described briefly and the supplementary results are shown.

II. Problem and notations

We investigate the structure of a stationary normal shock wave in a hard-sphere molecular gas. The flow is in the $X_1$ direction, where $X_i$ are the space rectangular coordinates. The $\rho_0$, $U_0$, $T_0$, and $M = (5kT_0/3m)^{-1/2}U_0$ are the density, flow speed, temperature,
and Mach number of the gas at upstream \( (X_1 = -\infty) \), respectively, where \( k \) and \( m \) are the Boltzmann constant and mass of the molecule, respectively; \( X_i = (\sqrt{\pi} l_0/2)x_i \); \( l_0 \) is the mean free path of gas molecules at upstream (for a hard-sphere molecular system, \( l_0 = [\sqrt{2\pi} \sigma^2 (\rho_0/m)]^{-1} \), where \( \sigma \) is the diameter of molecule); \( (2kT_0/m)^{1/2}\zeta_i \) is the molecular velocity; \( \rho_0(2\pi k T_0/m)^{-3/2}f(x_i, \zeta_i) \) is the velocity distribution function of the gas molecules; \( \rho_0 \rho, (2RT_0)^{1/2}u_1, T_0 T, p_0 P, p_0 (P \delta_{ij} + P_{ij}) \), and \( p_0 (2kT_0/m)^{1/2}Q_i \) are the density, flow velocity, temperature, pressure, stress tensor, and heat flow vector of the gas, respectively, where \( \delta_{ij} \) is the Kronecker delta.

### III. Formulation

The nondimensional Boltzmann equation in the present case is written as

\[
\zeta_1 \frac{\partial f}{\partial x_1} = G[f, f] - \nu[f]f,
\]

\( (1) \)

\[
G[f, g](x_1, \zeta_i) = \int f(x_1, \zeta_i + \alpha_i (V_j \alpha_j))g(x_1, \xi_i - \alpha_i (V_j \alpha_j))
\times B(|V_j \alpha_j|, V) d\Omega(\alpha_i) d\xi_1 d\xi_2 d\xi_3,
\]

\( (2) \)

\[
\nu[f](x_1, \zeta_i) = \int f(x_1, \xi_i) B(|V_i \alpha_i|, V) d\Omega(\alpha_i) d\xi_1 d\xi_2 d\xi_3,
\]

\( (3) \)

where \( V_i = \xi_i - \zeta_i \), \( V = |V_i| \), \( \alpha_i \) is a unit vector, \( d\Omega(\alpha_i) \) is the solid angle element in the direction of \( \alpha_i \), and \( B \) is given by

\[
B(|V_i \alpha_i|, V) = \frac{1}{4\sqrt{2\pi}^2} |V_i \alpha_i|,
\]

\( (4) \)

for hard-sphere molecules. The domain of the integration with respect to \( \zeta_i \) and \( \alpha_i \) is the whole space and all direction.

The nondimensional macroscopic variables are given by the moments of \( f \):

\[
\rho = \frac{1}{\pi^{3/2}} \int f d\zeta_1 d\zeta_2 d\zeta_3,
\]

\( (5a) \)

\[
u_i = \frac{1}{\pi^{3/2} \rho} \int \zeta_i f d\zeta_1 d\zeta_2 d\zeta_3,
\]

\( (5b) \)

\[
T = \frac{2}{3\pi^{3/2} \rho} \int (\zeta_i - \nu_i)^2 f d\zeta_1 d\zeta_2 d\zeta_3,
\]

\( (5c) \)
\[ P = \rho T, \]  
\[ P_{ij} = \frac{2}{\pi^{3/2}} \int (\zeta_{i} - u_{i})(\zeta_{j} - u_{j}) f d\zeta_{1} d\zeta_{2} d\zeta_{3} - P \delta_{ij}, \]  
\[ Q_{i} = \frac{1}{\pi^{3/2}} \int (\zeta_{i} - u_{i}) (\zeta_{j} - u_{j})^{2} f d\zeta_{1} d\zeta_{2} d\zeta_{3}. \]

The boundary condition at upstream and downstream is

\[ f \rightarrow \exp\left[-(\zeta_{1} - \sqrt{5/6}M)^{2} - \zeta_{2}^{2} - \zeta_{3}^{2}\right] \quad (x_{1} \rightarrow -\infty), \]  
\[ f \rightarrow \rho_{d} T_{d}^{-3/2} \exp\left[-\{ (\zeta_{1} - u_{d})^{2} + \zeta_{2}^{2} + \zeta_{3}^{2}\}/T_{d}\right] \quad (x_{1} \rightarrow \infty), \]

where \( \rho_{d}, u_{d}, \) and \( T_{d} \) are given by the Rankine-Hugoniot relation\( \dagger \):

\[ \rho_{d} = 4M^{2}/(M^{2} + 3), \]  
\[ u_{d} = \sqrt{5/96}(M^{2} + 3)/M, \]  
\[ T_{d} = (5M^{2} - 1)(M^{2} + 3)/16M^{2}. \]

**IV. Numerical method**

The distribution function in the form of \( f = f(x_{1}, \zeta_{1}, \zeta_{r}), \zeta_{r} = (\zeta_{2}^{2} + \zeta_{3}^{2})^{1/2} \), is compatible with the present problem. We solve the Boltzmann equation (1) for \( f(x_{1}, \zeta_{1}, \zeta_{r}) \) numerically by an iterative finite difference scheme. In this scheme, the \( \partial f/\partial x_{1} \) term is replaced by the standard central finite difference and the collision term is computed directly using the *numerical kernel* in the following way. Let \( \zeta_{1}^{(i)} \) be the lattice point of \( \zeta_{1} \) and \( \zeta_{r}^{(j)} \) be that of \( \zeta_{r} \). We first expand \( f \) in terms of \( \zeta_{1} \) in a similar way to the finite element method:

\[ f(\zeta_{1}, \zeta_{r}) = \sum_{i=-N_{m}}^{N_{p}} f(\zeta_{1}^{(i)}, \zeta_{r}) \Psi_{i}(\zeta_{1}), \]  
\[ \dagger \] Equation (7) is also derived from the conservation law of the Boltzmann equation (1).
and below the space variable $x_1$ is omitted for short). Next, we expand $f(\zeta_1^{(i)}, \zeta_r)$ by the sequence of the Laguerre polynomials of $\zeta_r^2$:

$$f(\zeta_1^{(i)}, \zeta_r) = \sum_{j=0}^{H-1} a_{ij} L_j(\zeta_r^2) \exp(-\zeta_r^2/2),$$

(9)

where $L_j(x)$ is the Laguerre polynomial of degree $j$. The expansion coefficient $a_{ij}$ is given by

$$a_{ij} = 2 \int_0^\infty f(\zeta_1^{(i)}, \zeta_r) L_j(\zeta_r^2) \zeta_r \exp(-\zeta_r^2/2) d\zeta_r.$$  

(10)

We introduce $\zeta_r$ lattice system defined by $L_H[(\zeta_r^{(j)})^2] = 0$ and compute $a_{ij}$ from the values of $f(\zeta_1^{(i)}, \zeta_r^{(k)}) \exp[(\zeta_r^{(k)})^2/2], k = 1, \cdots, H$, using Gauss-Laguerre quadrature. Combining Eqs. (8) and (9) and arranging the result in the order of power of $\zeta_r$, i.e.,

$$f(\zeta_1, \zeta_r) = \sum_{i=-N_m}^{N_p} \sum_{j=0}^{H-1} A_{ij} \Psi_i(\zeta_1) \zeta_r^{2j} \exp(-\zeta_r^2/2),$$

(11)

and substituting Eq. (11) into Eqs. (2) and (3), we have

$$G[f, f](\zeta_1 = \zeta_1^{(i)}, \zeta_r = \zeta_r^{(j)}) = \sum_{p=-N_m}^{N_p} \sum_{q=-N_m}^{N_p} \sum_{a=0}^{H-1} \sum_{b=0}^{H-1} \Omega_{pqab}^{ij} A_{pa} A_{qb},$$

(12)

$$\nu[f](\zeta_1 = \zeta_1^{(i)}, \zeta_r = \zeta_r^{(j)}) = \sum_{p=-N_m}^{N_p} \sum_{a=0}^{H-1} \Lambda_{pa}^{ij} A_{pa},$$

(13)

where

$$\Omega_{pqab}^{ij} = G[\Psi_p(\zeta_1)\xi_r^{2a} E_r, \Psi_q(\zeta_1)\xi_r^{2b} E_r](\zeta_1 = \zeta_1^{(i)}, \zeta_r = \zeta_r^{(j)}),$$

(14)

$$\Lambda_{pa}^{ij} = \nu[\Psi_p(\zeta_1)\xi_r^{2a} E_r](\zeta_1 = \zeta_1^{(i)}, \zeta_r = \zeta_r^{(j)}),$$

(15)

with

$$E_r = \exp(-\xi_r^2/2).$$

The complexity of the collision term appears only in the numerical kernel $\Omega_{pqab}^{ij}$ and $\Lambda_{pa}^{ij}$, which can be computed in advance and are stored. In order to reduce the number of elements of numerical kernel, a uniform $\zeta_1$ lattice system is introduced, i.e., $\zeta_1^{(i)} = i\Delta$. 

Then, from the relation of the collision operator for the translation and mirror image, we have

\[ \Omega_{pqab}^{ij} = \Omega_{p^{-i},q^{-i},ab}^{0,j}, \quad \Lambda_{pa}^{ij} = \Lambda_{p^{-i},a}^{0,j}, \quad (16) \]

\[ \Omega_{pqab}^{0,j} = \Omega_{-p,-q,ab}^{0,j}, \quad \Lambda_{pa}^{0,j} = \Lambda_{-p,a}^{0,j}. \quad (17) \]

Furthermore, for hard-sphere molecules the following relation holds:

\[ \Omega_{pqab}^{0,j} = \Omega_{qpba}^{0,j}, \quad \Omega_{pqab}^{0,j} = \Omega_{pqba}^{0,j}. \quad (18) \]

Owing to Eqs. (16)-(18) we can reduce the total number of the elements from \((N_m + N_p + 1)^3 H^3\) to about \((3/8)(N_m + N_p + 1)^2 H^3\). Each element of the numerical kernel, generally expressed by a five fold integral, can be reduced to two fold one in the case of hard-sphere molecules and is computed accurately\(^{11}\); if we expand \(f\) in terms of \(\zeta_r\) by a set of basis function, the effective domain of integration of the numerical kernel becomes geometrically very complicated.

The present method is based on the form of the similarity solution (see Ref. 12 for the linearized Boltzmann equation). The numerical kernel method for general form of the distribution function, though the lattice system which can be used in the actual computation is limited to very coarse one at the present stage, has been proposed by Tan, et. al in Ref. 13.

V. Result and discussion

In Ref. 11, the numerical results are presented for \(M = 1.2 \sim 3\) together with several accuracy data of computation. In the present study, we supplement the results for \(M = 1.1\) and 3.2.

The computation was carried out using the numerical kernel in Ref. 11 [(M3) molecular velocity lattice system, i.e., 101 lattice points for \(\zeta_1 (\Delta = 0.15)\) and 14 lattice points for \(\zeta_r (H = 14, \zeta_r^{(H)} = 6.6607\ldots)\)]. In the case of \(M = 1.1\), we computed \(\overline{f}(x_1, \zeta_1, \zeta_r) = f(x_1, \zeta_1/\sqrt{2}, \zeta_r/\sqrt{2})\) in stead of \(f\), since the distribution function is almost upstream
Maxwellian, i.e., \( f(x_1, \zeta_1, \zeta_r) \sim \exp(-\zeta_1^2 - \zeta_r^2) \), and therefore, \( \bar{f} \sim \exp[-\zeta_r^2/2] \), and the leading term of the Laguerre polynomial expansion is proportional to \( \exp[-\zeta_r^2/2] \). The space interval is \(-70 \leq x_1 \leq 70\) for \( M = 1.1 \) and \(-20 \leq x_1 \leq 20\) for \( M = 3.2 \). The space lattice system is uniform for \( M = 1.1 \) (100 sections) and nonuniform for \( M = 3.2 \) [(S2) system in Ref. 11, i.e., 100 sections with the minimum width 0.100 around \( x_1 = 0 \) and maximum one 1.283 around \( x_1 = \pm 20 \)]. The numerical results satisfy the conservation law, the constancy of mass, moment, and energy fluxes at all the space lattice points, within the range of 0.03% for \( M = 1.1 \) and 0.05% for \( M = 3.2 \). For the comparison, we also carried out the Monte-Carlo direct simulation using Bird’s NTC method and the piston boundary condition at down stream\(^8\) [Hard-Sphere, \( M = 3.2 \), \(-20 \leq x_1 \leq 20\), 100 uniform cells, about 32500 particles, 8000 samples].

The \( \rho, u_1, \) and \( T \) vs. \( x_1 \) for \( M = 1.1 \) are tabulated in Table I together with those of the asymptotic solution for weak shock\(^{11}\), which is derived up to \( O(\epsilon^2) \), (\( \epsilon = M - 1 \)), by the \( \epsilon \) expansion of \( f \) around upstream Maxwellian under the assumption that the shock thickness is \( O(l_0/\epsilon) \) [see Appendix]. The present numerical result agrees very well with the asymptotic solution. The normalized density \( \bar{\rho} = \rho/(\rho(\infty) - 1) \), flow speed \( \bar{u}_1 = u_1/(u_1(-\infty) - u_1(\infty)) \), and temperature \( \bar{T} = T/(T(\infty) - 1) \) vs. \( x_1 \) for \( M = 3.2 \) are plotted in Fig.1 together with the Mott-Smith solution corresponding to the moment equation of \( \int \zeta_1^3 f d\zeta_1 \zeta_2 \zeta_3 \) and the DSMC result. In Fig.2 the results of these methods are compared at the distribution function level. Although the difference between the Mott-Smith solution and the present result is slight at the macroscopic level, there is a distinct difference at the microscopic level. The standard deviation of the samples of simulation for the density is not small, nevertheless, the average of samples agrees very well with the present result at the microscopic level as well, which shows the averaging procedure works quite well.

We analyzed the structure of normal shock waves up to moderate strength numerically with good accuracy. In the case of strong shock wave (the temperature difference in the gas is large), many terms is required in the Laguerre polynomial expansion for the
accurate computation. However, it becomes very difficult to compute $\Omega_{pqab}^{0,k}$ accurately for large $a$ and $b$. The application range of the present method is practically limited up to moderate shock strength.

Appendix: Analysis of weak shock waves

A. Outline of analysis

The analysis is carried out in a similar way to the Hilbert expansion. We introduce a new space coordinate $\eta = \epsilon x_1$, where $\epsilon = M - 1$. For the convenience of analysis, we use the following independent variables and function: $(\hat{\zeta}_1, \hat{\zeta}_2, \hat{\zeta}_3) = (\zeta_1 - \sqrt{5/6}M, \zeta_2, \zeta_3)$, $\hat{\zeta} = (\hat{\zeta}_i^2)^{1/2}$, $\hat{f}(\eta, \hat{\zeta}_1, \hat{\zeta}_2, \hat{\zeta}_3) = f(x_1, \zeta_1, \zeta_2, \zeta_3)$. Then the Boltzmann equation (1) for $\hat{f}$ is written as

$$(\hat{\zeta}_1 + \sqrt{5/6}M) \frac{\partial \hat{f}(\eta, \hat{\zeta}_i)}{\partial \eta} = \frac{1}{\epsilon} Q[\hat{f}, \hat{f}](\eta, \hat{\zeta}_i),$$

where

$$Q[\hat{f}, \hat{g}] = \frac{1}{2} (G[\hat{f}, \hat{g}] + G[\hat{g}, \hat{f}] - \nu[\hat{f}] \hat{g} - \nu[\hat{g}] \hat{f}).$$

We expand $\hat{f}$ into a power series of $\epsilon$ around the upstream Maxwellian $\hat{f}_0 = \exp(\hat{\zeta}^2)$:

$$\hat{f}(\eta, \hat{\zeta}_i) = \hat{f}_0 [1 + \phi_1(\eta, \hat{\zeta}_i) \epsilon + \phi_2(\eta, \hat{\zeta}_i) \epsilon^2 + \cdots].$$

Substituting Eq.(A2) into Eq.(A1) and assuming $\partial \phi_i / \partial \eta = O(1)$, i.e., $\delta/l_0 = O(1/\epsilon)$, and arranging the result in the order of power of $\epsilon$, we have the following sequence of linear integral equations:

$$2Q[\hat{f}_0, \hat{f}_0 \phi_1] = 0,$$

$$2Q[\hat{f}_0, \hat{f}_0 \phi_2] = (\hat{\zeta}_1 + \sqrt{5/6}) \hat{f}_0 \frac{\partial \phi_1}{\partial \eta} - Q[\hat{f}_0 \phi_1, \hat{f}_0 \phi_1],$$

$$2Q[\hat{f}_0, \hat{f}_0 \phi_n] = (\hat{\zeta}_1 + \sqrt{5/6}) \hat{f}_0 \frac{\partial \phi_{n-1}}{\partial \eta} + \sqrt{5/6} \hat{f}_0 \frac{\partial \phi_{n-2}}{\partial \eta} - \sum_{1+\ell=1, 1+m=n} Q[\hat{f}_0 \phi_1, \hat{f}_0 \phi_m] \quad (n \geq 3).$$

(A3c)
The boundary condition (16) is expanded in a similar way to Eq.(A2). The integral equations are, in principle, solved from the lowest order. The homogeneous integral equation [(A3a)] has nontrivial solutions \( \{1, \hat{\zeta}_1, \hat{\zeta}^2\} \) and the coefficient functions of \( \{1, \hat{\zeta}_1, \hat{\zeta}^2\} \) in \( \phi_n \), functions of \( \eta \), are determined by the solvability conditions of \((n+1)th\) and \((n+2)th\) integral equations and the boundary condition for \( \phi_n \). The position of solution is arbitrary in this problem and we determine it in such a way that the density corresponding to \( \hat{f}_0 \phi_n \), \( \rho^n(\eta) \), satisfies \( \rho^n(0) = [\rho^n(-\infty) + \rho^n(+\infty)]/2 \).

B. Result

We show the results up to \( O(\epsilon^2) \) below. The distribution function is

\[
\phi_1 = a(\eta)(-\sqrt{15/2}\hat{\zeta}_1 + \hat{\zeta}^2),
\]

\[
\phi_2 = b_1(\eta) + b_2(\eta)\hat{\zeta}_1 + b_3(\eta)\hat{\zeta}^2
\]

\[
+ a(\eta)^2[-\sqrt{15/2}\hat{\zeta}_1(\hat{\zeta}^2 - 5/2) + (15/4)(\hat{\zeta}_1^2 - \hat{\zeta}^2/3) + (1/8)(4\hat{\zeta}^4 - 20\hat{\zeta}^2 + 15)]
\]

\[
+ \sqrt{30}\lambda_1^{-1}\exp(-\sqrt{30}\eta/\lambda_1)a(\eta)^2[\sqrt{15/8}(\hat{\zeta}_1^2 - \hat{\zeta}^2/3)B(\hat{\zeta}) - \hat{\zeta}_1A(\hat{\zeta})],
\]

(A4b)

where

\[
a(\eta) = (1 + \exp(-\sqrt{30}\eta/\lambda_1))^{-1},
\]

\[
b_1(\eta) = (15/2)a(\eta)[-\lambda_4 + (\lambda_4 - 1/2)a(\eta)],
\]

\[
b_2(\eta) = \sqrt{15/2}[-b_3(\eta) + a(\eta)\{5\lambda_4 - 1 - (5\lambda_4 - 5/2)a(\eta)\}],
\]

(A5)

\[
b_3(\eta) = a(\eta)^2\left[5/2 + \exp(-\sqrt{30}\eta/\lambda_1)\{\lambda_2\eta + \lambda_3\log[1 + \exp(\sqrt{30}\eta/\lambda_1)] + \lambda_5\}\right],
\]

\[
\lambda_1 = (2\gamma_1 + \gamma_2), \quad \lambda_2 = \sqrt{15/2}[-8(\gamma_1^2 + \gamma_2^2 - \gamma_5)/\lambda_1^3 + 1/\lambda_1],
\]

\[
\lambda_3 = -(20\gamma_1\gamma_2 + 8\gamma_5)/\lambda_1^2 + (14\gamma_1 + 13\gamma_2 - 2\gamma_4 - \gamma_5)/\lambda_1 - 11/2,
\]

\[
\lambda_4 = \gamma_2/\lambda_1, \quad \lambda_5 = 5\lambda_4 - \lambda_3\log 2.
\]

(A6)

The \( A(\hat{\zeta}) \) and \( B(\hat{\zeta}) \) are the solution of the following integral equations:

\[
2Q[\hat{f}_0\hat{\zeta}_1 A(\hat{\zeta}), \hat{f}_0] = -\hat{f}_0\hat{\zeta}_1(\hat{\zeta}^2 - 5/2),
\]

\[
\int_0^\infty \hat{\zeta}^4 A(\hat{\zeta})\exp(-\hat{\zeta}^2)d\hat{\zeta} = 0,
\]

(A7)
$2Q[\hat{f}_0(\hat{\zeta}_1^2 - \hat{\zeta}^2/3)B(\hat{\zeta}), \hat{f}_0] = -2\hat{f}_0(\hat{\zeta}_1^2 - \hat{\zeta}^2/3)$, \hspace{1cm} (A8)

and $\gamma_i$ are constants given by

\begin{align*}
\gamma_1 &= I_6(B), \quad \gamma_2 = 2I_6(A), \quad \gamma_3 = I_6(AB), \\
\gamma_4 &= -(5/2)\gamma_1 + I_8(B) + (1/2)I_6(BC), \quad \gamma_5 = -6\gamma_2 + 2I_8(A) + 2I_4(AG), \hspace{1cm} (A9) \\
\gamma_s &= (5/2)I_4(A^2) + (5/4)I_6(AB), \gamma_s = -(5/2)I_4(A^2) + (5/4)I_6(AB) - 2\gamma_3,
\end{align*}

where

$$I_n(F) = (8/15) \pi^{-1/2} \int_0^\infty \hat{\zeta}^n F(\hat{\zeta}) \exp(-\hat{\zeta}^2) d\hat{\zeta},$$

and $C(\hat{\zeta})$ and $G(\hat{\zeta})$ are defined by

\begin{align*}
2Q[\hat{f}_0 \hat{\zeta}^2, \hat{f}_0 \hat{\zeta}_1 A(\hat{\zeta})] &= \hat{f}_0(\hat{\zeta}_1^2 - \hat{\zeta}^2/3)(C(\hat{\zeta}) - 3), \hspace{1cm} (A10) \\
2Q[\hat{f}_0 \hat{\zeta}^2, \hat{f}_0 \hat{\zeta}_1 A(\hat{\zeta})] &= \hat{f}_0(\hat{\zeta}_1^2 - \hat{\zeta}^2/3)(C(\hat{\zeta}) - 3), \hspace{1cm} (A11)
\end{align*}

The macroscopic quantities corresponding to the above distribution function are

\begin{align*}
\rho &= 1 + (3/2)a(\eta)\varepsilon + [b_1(\eta) + (3/2)b_3(\eta)]\varepsilon^2 + \cdots, \\
u_1 &= \sqrt{5/6} + [\sqrt{5/6} - \sqrt{15/8}a(\eta)]\varepsilon + [b_2(\eta)/2 + \sqrt{135/32}a(\eta)^2]\varepsilon^2 + \cdots, \\
T &= 1 + a(\eta)\varepsilon + [b_3(\eta) - (11/4)a(\eta)^2]\varepsilon^2 + \cdots, \hspace{1cm} (A12) \\
P_{11} &= -2P_{22} = -2P_{33} = 10\gamma_1\lambda_1^{-1}\exp(-\sqrt{30}\eta/\lambda_1)a(\eta)^2\varepsilon^2 + \cdots, \\
Q_1 &= -(5/4)\sqrt{30}\gamma_2\lambda_1^{-1}\exp(-\sqrt{30}\eta/\lambda_1)a(\eta)^2\varepsilon^2 + \cdots.
\end{align*}

The accurate numerical data of $A(\hat{\zeta})$ and $B(\hat{\zeta})$ for hard-sphere molecules were first obtained by Pekeris and Alteman and the recomputed data are tabulated in Ref.16. The quantities of $\gamma_i$ for hard-sphere molecules are

\begin{align*}
\gamma_1 &= 1.270042427, \quad \gamma_2 = 1.922284066, \quad \gamma_3 = 1.947906335, \\
\gamma_4 &= 0.635021214, \quad \gamma_5 = 0.961142033, \quad \gamma_s = 4.893662449.
\end{align*}

It should be noted that the above results up to $O(\varepsilon^2)$ are derived from Burnett solution in Chapman-Enskog theory when the macroscopic variables are expanded in a similar way.
References


Table I. The density \( \rho \), flow velocity \( u_1 \), and temperature \( T \) vs. \( x_1 \) for \( M = 1.1 \).

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The results are shifted for \( x_1 \) in such a way that the point with average density is located at \( x_1 = 0 \). The data for the present numerical computation are interpolated with sufficient accuracy from those at the lattice points.
Fig. 1. The profiles of normalized density $\tilde{\rho}$, flow velocity $\tilde{u}_1$, and temperature $\tilde{T}$ vs. $x_1$ for $M = 3.2$. Here, indicates the present numerical result, the Mott-Smith\(^1\), and o, x, and + are $\tilde{\rho}$, $\tilde{u}_1$, and $\tilde{T}$ of the DSMC result, respectively. The results are shifted for $x_1$ in such a way that the point with average density is located at $x_1 = 0$. The length of each vertical line shows the magnitude of the standard deviation of the DSMC samples for the density at the corresponding point.

$\tilde{\rho}, \tilde{u}_1, \tilde{T}$

$-8$ $-4$ $0$ $4$ $8$

$x_1$

Fig. 1a. Distribution function $f(x_1, \zeta_1, \zeta_r)$ for $x_1 = -0.554$ and different values of $\zeta_r$.
Fig. 2. Comparison of the distribution function $f(x_1, \zeta_1, \zeta_r)$ for $M = 3.2$ at (a) $x_1 = -0.554$, (b) $x_1 = 0.646$, and (c) $x_1 = 1.446$. Here, ———— indicates the present numerical result, ———— the Mott-Smith, and $\circ$, $\Box$, $\times$, and + are the DSMC result corresponding to $\zeta_r = 0.15, 0.75, 1.35$, and $1.95$, respectively. The results are shifted for $x_1$ in such a way that the point with average density is located at $x_1 = 0$. 