STRUCTURE OF A SHOCK WAVE IN A SIMPLE MONATOMIC GAS

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STRUCTURE OF A SHOCK WAVE IN A SIMPLE MONATOMIC GAS

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The determination of the structure of a plane shock discontinuity in a simple monatomic Boltzmann gas, in a rigorous formulation, reduces to solving the Boltzmann kinetic equation (1) with boundary conditions (2)

$$\xi \, \partial f/\partial x = I[f]; \tag{1}$$

$$\vec{f}(\xi, x = -\infty) = f_0(\vec{\xi}; n_1, u_1, T_1), \tag{2}$$

$$f(\vec{\xi}, x = +\infty) = f_0(\vec{\xi}; n_2, u_2, T_2),$$

where

$$f_0 = n(m/2\pi T)^{1/2} \exp\{-m[(\xi - u)^2 + \eta^2 + \zeta^2]/2T\},$$

and ξ, η, ζ are the components of the vector $\vec{\xi}$.

The parameters $n_1, u_1, T_1, n_2, u_2, T_2$ are related by the Rankine–Hugoniot conditions. After the distribution function has been found, the macroscopic quantities—density, temperature, mean velocity, momentum and energy fluxes—can be calculated as the corresponding averages over velocity space.

The difficulty of solving problem (1)–(2) consists primarily in its high dimensionality. The necessity of computing the three-dimensional distribution function $f(\xi, \eta^2 + \zeta^2, x)$ leads to a large volume of information to be processed, while five-fold quadratures in the collision integral sharply increase the required number of machine operations.

Apparently, these difficulties explain the attempts to proceed without solving the kinetic equation, replacing it by simulating a certain random process that more or less plausibly models the phenomenon ($^{1-3}$), or by using, instead of the Boltzmann equation, a "relaxation" kinetic equation close to it in physical meaning (^{4,5}).

We undertook an attempt to solve the problem in a rigorous formulation, based on the use of statistical considerations and counting methods, as well as an algorithm of successive approximations that does not require storing large arrays of the distribution function.

Absolutely elastic spheres of constant diameter σ were chosen as the molecular model. Such a model corresponds to the physical picture of a gas as an ensemble of spherically symmetric molecules with a constant effective collision cross section and possessing no internal degrees of freedom. The Boltzmann collision integral can be transformed to the form

$$I = -\nu f + N, \tag{3}$$

$$\nu[f_1] = 2\pi\sigma^2 \iiint_{-\infty}^{\infty} f_1 |q| \, d\xi_1 \, d\eta_1 \, d\zeta_1,$$

$$N[f' f_1'] = \pi^2\sigma^2 \int_0^1 \int_0^1 \iiint_{-\infty}^{\infty} f' f_1' |q| \sin(\pi\theta) \, d\theta \, d\varepsilon \, d\xi_1 \, d\eta_1 \, d\zeta_1, \tag{4}$$

where $|\mathbf{q}| = |\vec{\xi} - \vec{\xi}_1|$; $f' = f(\vec{\xi}')$, $f_1 \equiv f(\vec{\xi}_1)$, $f_1' \equiv f(\vec{\xi}_1')$; $\vec{\xi}' = \vec{\xi}'(\vec{\xi}, \vec{\xi}_1, \theta, \varepsilon)$, $\vec{\xi}_1' = \vec{\xi}_1'(\vec{\xi}, \vec{\xi}_1, \theta, \varepsilon)$; θ and ε are collision parameters.

To compute successive approximations, integral iterations of equation $(\cdots)$–(2) with allowance for (3) were used.

$$\begin{aligned} f^{(n)}(\xi > 0, x) &= f_0(\vec{\xi}; n_1, u_1, T_1) \exp\left\{-\frac{1}{\xi}\int_a^x \nu^{(n-1)}(\xi, x_1)\, dx_1\right\} \\ &\quad + \frac{1}{\xi}\int_a^x N^{(n-1)}(\xi, x_1) \exp\left\{-\frac{1}{\xi}\int_{x_1}^x \nu(\xi, x_2)\, dx_2\right\} dx_1, \\ f^{(n)}(\xi < 0, x) &= f_0(\vec{\xi}; n_2, u_2, T_2) \exp\left\{-\frac{1}{|\xi|}\int_x^b \nu^{(n-1)}(\xi, x_1)\, dx_1\right\} \\ &\quad + \frac{1}{|\xi|}\int_x^b N^{(n-1)}(\xi, x_1) \exp\left\{-\frac{1}{|\xi|}\int_{x_1}^x \nu(\xi, x_2)\, dx_2\right\} dx_1. \end{aligned} \tag{5}$$

Here $f^{(n)}$ is the distribution function computed in the n-th iteration; $\nu^{(n-1)}$, $N^{(n-1)}$ are the values of the integrals ν and N containing the distribution function in the $(n-1)$-st approximation. The boundary conditions at $-\infty$ and $+\infty$ are transferred to sufficiently large distances $-a$ to the left and $+b$ to the right

Fig. 1. Flow velocity and gas temperature in a shock wave. 1—Boltzmann equation, 2—relaxation equation

Figure 1: Fig. 1. Flow velocity and gas temperature in a shock wave. 1—Boltzmann equation, 2—relaxation equation

of the notional center of the jump, determined by the position of the initial gas-dynamic discontinuity.

Since the macroscopic quantities are defined as mean values of the distribution function, it proved possible to compute it at each phase point $(\vec{\xi}, x)$ only with statistical accuracy, which made it possible to compute the integrals ν and N by the Monte Carlo method with a small number of trials. The integral scheme (5) proved sufficiently stable for such computations.

Fig. 1. Flow velocity and gas temperature in a shock wave. 1—the Boltzmann equation, 2—the relaxation equation

To determine $f^{(n)}(\vec{\xi}, x)$ at a prescribed phase point $(\vec{\xi}, x)$, random numbers $(\vec{\xi}_1, \theta, \varepsilon)$ were drawn at a number of points $x_i > x$ for $\xi < 0$ or $x_i < x$ for $\xi > 0$, determining the argument $f^{(n-1)}(\vec{\xi}_1, x_i)$ in the integral $\nu^{(n-1)}$, and the values $\vec{\xi}'$ and $\vec{\xi}_1'$ entering into the argument $f^{(n-1)}$ and $f_1^{(n-1)}$ in the integral $N^{(n-1)}$ were computed; for each phase point $(\vec{\xi}_1', x_i)$, $(\vec{\xi}', x_i)$ obtained in this way, random numbers determining the argument of the functions $f^{(n-2)}$, etc., were in turn drawn.

The diagram of computations constructed in this way is a tree, each vertex of which is determined by the value of the random vector $(\vec{\xi}, x)$ in only one preceding vertex. This makes it possible not to store in advance all vertices $(\vec{\xi}_k, x_k)$, which would be difficult, but to carry out such draws in the course of the computations along each branch of the iteration tree.

However, as the order of approximation increases, the number of vertices at which the first iteration $f^{(1)}$ must be computed grows avalanche-like, and with it the computation time increases.

On the BESM-6 computer of the Computing Center of the USSR Academy of Sciences, it proved possible to carry out three successive iterations.

Fig. 2
Fig. 2. Change of entropy in a shock wave. 1 —Boltzmann entropy, 2 —thermodynamic entropy

Fig. 3
Fig. 3. Longitudinal $T_\parallel$ and transverse $T_\perp$ gas temperature in a shock wave

For constructing the zeroth iteration, the boundary-value problem (2) was first solved for the relaxation kinetic equation with a collision frequency corresponding to the adopted molecular model. The solution obtained, $f_r(\vec{\xi}, x)$, at each point x was approximated locally by the Maxwellian function $f_0(\vec{\xi}; n, u, T)$, with values of the parameters n, u, T determined by the function $f_r(\vec{\xi}, x)$. This approximation made it possible to reduce substantially the computations of $f^{(1)}$.

Fig. 4

Fig. 4. Profiles of the distribution function $f(\xi, 0, 0, x)$ in a shock wave

To prove the convergence of the iterations, first, the equation of conservation of the mass flux in a plane shock wave was used. In the third iteration the deviation from the true value was 2%, whereas in the second it was 4.5%. Second, integration was carried out (the circles in Fig. 1), starting from another initial profile $n(x), u(x), T(x)$, namely the one obtained in the first iteration of the Boltzmann equation. Figures 1-4 present the results of the calculation for $M = 2$. The profiles $u(x)$ and $T(x)$ (Fig. 1) differ little from the profiles obtained from the relaxation kinetic equation.

Figure 2 shows the change of entropy $S = -\frac{1}{n}\int f \ln f \, d\vec{\xi}$ and of the thermodynamic entropy $S_0 = c_v \ln(p/\rho^\gamma)$. A curious feature of the behavior of the quantity S is the presence of a small local minimum to the right of the middle of the jump. It might have been attributed to computational inaccuracy; however, a similar minimum (though shifted somewhat along the x-axis) is also found in the solution of the relaxation equation, where the accuracy of the computations is no worse than 0.5%.

As is seen from Fig. 3, the gas in the shock wave has two substantially different temperatures of the translational degrees of freedom; pro-

longitudinal temperature

$$T_\parallel = \frac{1}{n}\int (\xi - u)^2 f \, d\vec{\xi}$$

and transverse temperature

$$T_\perp = \frac{1}{2n}\int (\eta^2 + \zeta^2) f \, d\vec{\xi}.$$

Figure 4 gives profiles of the distribution function $f(\xi, 0, 0, x)$, calculated at three points inside the shock layer. The values of x are referred to the mean free path in the gas to the left of the discontinuity, $\lambda = 1/\sqrt{2}\Delta\sigma^2 n_1$; the values of T and u are referred respectively to T_1 and $u_0 = \sqrt{T_1/m}$.

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