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In the hydrodynamics of an ideal fluid a shock wave is a geometrical surface of a discontinuity of hydrodynamical (and thermodynamical) quantities. Introducing viscosity and thermal conductivity into the equations of hydrodynamics changes both the pattern of origin of the shock wave and also its structure. A transition layer of finite width appears instead of a geometrical discontinuity surface (we note the obvious arbitrariness of the concept of the "width" of the transition layer, in view of the asymptotic nature of change of state of the medium at its "boundaries"). For shock waves which are weak enough the Navier-Stokes equations apply to the flow in the transition layer and thus fully determine its structure (see, for example, [1]). However, in the case of strong shock waves in a gas (by this we understand shock waves in which the difference of the densities at the boundaries of the transition layer. for example, is a quantity of the same order as the values of the densities themselves) an estimate of the width Δx of the shock wave by means of the Navier-Stokes equations leads to the result

$$\Delta x \approx l_0 \tag{1}$$

where t_0 is the gas molecule free path [1] (here the transport coefficients are expressed in terms of molecular quantities). The equations of macroscopic gas dynamics are inapplicable to processes in such regions of space, and the width of the transition layer (1) in the macroscopic treatment should be set equal to zero. Thus, an estimate of the width of the shock wave by the methods of the kinetic theory of gases is of widespread interest. Below we make such an estimate directly with the help of Boltzmann's kinetic equation and his H-theorem (without having recourse to solving the kinetic equation).

Thus, within the framework of the phenomenological description. a shock wave of great intensity is a geometrical surface of discontinuity on both sides of which the flow may be described by the equations of gas dynamics, containing viscosity and thermal conductivity coefficients. but dissipative processes localized in the "surface" of discontinuity make the basic contribution to the increase of entropy of the medium. From the point of view of molecular kinetics these processes evolve in a thin layer of gas which is in a markedly nonequilibrium state. First of all, we shall restrict outselves to the case of a shock wave in a monatomic gas ("structureless" particles). Then the state of the gas in the layer under consideration may be described by means of a distribution function $f(\mathbf{c}, \mathbf{r}, t)$, where \mathbf{r} is the position vector of the molecule, and c its velocity. The expression f(c, r, t) dr dcgives the number of molecules in the element dr of coordinate space and the element dc of velocity space in the neighborhood of the points r and c, respectively.

In the case of a strong shock wave the function f varies substantially over the width of the layer. Under these circumstances the entropy cannot be determined thermodynamically in the layer as a whole or in its elements. Moreover, we cannot apply the concept of entropy production here in the same form as that in which it is introduced in the thermodynamics of irreversible processes [2], since here a thermodynamic description of nonequilibrium systems is assumed. However, both these concepts may be extended to a system with a nonequilibrium distribution function H with the help of Boltzmann's H-function. The local value of the generalized entropy H per unit volume is determined by the following equation (see. for example, [3]):

$$H = -k \int \ln f \cdot f \, d\mathbf{c} \tag{2}$$

where k is Boltzmann's constant and the integration is performed over all velocity space. 1 For an equilibrium distribution function H coincides with the thermodynamic entropy.

Differentiating (2) with respect to time and representing the derivative $\partial f/\partial t$ by the expression from Boltzmann's equation (in the absence of external forces)

$$\frac{\partial f}{\partial t} + \mathbf{c} \frac{\partial f}{\partial \mathbf{r}} = \left(\frac{\partial f}{\partial t}\right)_{e} \tag{3}$$

leads to the relation

$$\frac{\partial H}{\partial t} + \operatorname{div} \mathbf{S} = \mathbf{s} \,. \tag{4}$$

Here $(\partial f/\partial t)_e$ is the collision integral representing the rate of change of the distribution function as a result of intermolecular collisions, and the following notation has been introduced

$$S = -k \int \mathbf{c} \ln f \cdot f \, d\mathbf{c} \,, \tag{5}$$

$$\sigma = -k \int (1+\ln f) \left(\frac{\partial f}{\partial t}\right)_e d\mathbf{c} \,. \tag{6}$$

The interpretation of equation (4) and expressions (5) and (6) is obvious. The vector S is the flux density vector of the generalized entropy, and σ is the entropy production—the change of generalized entropy per unit volume as a result of irreversible volume processes. Boltzmann showed that σ is positive for nonequilibrium gases and zero in the case of statistical equilibrium

$$s \ge 0$$
. (7)

Definition (2) and relations (4)-(7), together with the proof to which they give rise concerning the monotonic increase of entropy (generalized) of an isolated system, comprise the content of Boltz-mann's H theorem. We shall use these results to evaluate the width of the transition layer for strong shock waves.

We shall now consider the flow in a coordinate system relative to which the shock wave is motionless, and we shall take the velocity of the stream to be directed along the x axis. Assuming steady-state flow and integrating both sides of equation (4) with respect to x, we obtain

$$S_2 - S_1 = \int_{-\infty}^{+\infty} \sigma \, dx \tag{8}$$

where S_1 and S_2 are the values of the entropy flux density in the unperturbed and perturbed media, respectively.

The integral on the right-hand side of equation (8) is actually determined by a certain layer of finite width Δx , and equation (8) may be written in the form

$$S_2 - S_1 = \sigma^* \Delta x \tag{9}$$

where σ^* is some average value of the entropy production in the layer.

¹We take the molecules to be classical particles. For quantum particles whose motion is quasi-classical

$$H = k \int f \ln \frac{em^3}{fh^3} \, d\mathbf{c} \, .$$

Here h is Planck's constant, m is the mass of a molecule. e is the base of natural logs.

Equation (9) should be regarded as one of the possible definitions of shock wave width. We note that Δx depends on the choice of σ^* . The definition of Δx may be made unambiguous by taking σ^* as equal, for example, to the maximum value of the entropy production in the layer (σ being a positive quantity equal to zero at the "boundaries" of the layer). However, such refinements are unimportant for an order-ofmagnitude estimate of Δx .

We shall make an order-of-magnitude estimate of both sides of equation (9) using definitions (5) and (6). In so doing, we make use of the following estimates. For f we may take $f < c > ^3 \approx n$, where < c > is some average value of the thermal velocity, n is the particle number density. We assume that the variation of such quantities as (f), < c >, n, etc., on passing through the layer, are quantities of the same order as f, < c >, n, etc., respectively (a shock wave of high intensity). Thus, the left-hand side of equation (9) is equal in order of magnitude to

$$S_2 - S_1 \approx k \langle c \rangle \ln f \cdot f \langle c \rangle^3. \tag{10}$$

The collision integral $(\partial f/\partial t)_e$ has the form [3]

$$\left(\frac{\partial f}{\partial t}\right)_{e} = \iiint |\mathbf{c}_{1} - \mathbf{c}_{2}| (f'f_{1}' - ff_{1}) bdbd\varphi d\mathbf{c}_{1},$$
$$f_{1} \equiv f(\mathbf{c}_{1}), \quad f' \equiv f(\mathbf{c}'), \quad f_{1}' \equiv f(\mathbf{c}_{1}'). \tag{11}$$

Here c and c_1 are the velocities of the molecule before collision, c' and c'_1 are the velocities after collision, b is the impact parameter. φ is the angular collision parameter. When f departs appreciably from the Maxwellian distribution, we obtain from (11)

$$\left(\frac{\partial f}{\partial t}\right)_{e} \approx \langle c \rangle \frac{n^{2}}{\langle c \rangle^{6}} r_{0}^{2} \langle c \rangle^{3}$$
(12)

where r_0 is the effective radius of action of the intermolecular forces. Thus the right-hand side of equation (9) turns out to be equal in order of magnitude to

$$\approx k \ln f \langle c \rangle \langle c \rangle^3 \frac{n^3}{\langle c \rangle^6} r_0^2 \langle c \rangle^3 \Delta x.$$
 (13)

Setting estimates (10) and (13) in equation (9), we obtain

$$nr_0^2\Delta x\approx 1. \tag{14}$$

In order of magnitude the left-hand side of (14) is equal to the number of collisions experienced by a molecule on traversing the distance Δx . Thus it follows from (14) that Δx is of the order of the free path length, which agrees with estimate (1),

In the case of polyatomic gases relation (14) gives an estimate of the width of a thin transition layer with an appreciable departure from the Maxwellian velocity distribution (a shock "front" behind which there follows a relatively wide zone in which an equilibrium distribution of energy between internal and translational degrees of freedom is established). In this transition layer the gas practically behaves as though it were monatomic. Thus, all relations which led to estimate (14) apply here, too.

We note that the time for establishing equilibrium between the rotational and translational degrees of freedom is usually close in order of magnitude to the time of free motion (somewhat exceeding it). In this case the width of the corresponding zone may be estimated by means of a natural extension of the derivation explained here.

REFERENCES

1. L. D. Landau and E. M. Lifschitz, Mechanics of Continua [in Russian], Gostekhizdat, 1953.

2. S. DeGroot and P. Mazur. Nonequilibrium Thermodynamics [Russian translation], Izd. "Mir." 1964.

3. A. Sommerfeld, Thermodynamics and Statistical Physics [Russian translation], Izd. inostr. lit., 1955.

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