

## Shock waves in two-dimensional gas

M. BRATOS and R. HERCZYŃSKI (WARSZAWA)

THE TAMM variational method used to determine the shock wave structure is generalized to take into account different kinds of the intermolecular potential. A comparison of the results with available theoretical studies is presented.

Zastosowano wariacyjną metodę Tammy do badania wpływu potencjału oddziaływania międzymolekularnego na strukturę fali uderzeniowej. Uzyskane wyniki numeryczne porównano z innymi teoretycznymi wynikami.

Применен вариационный метод Тамма для исследования влияния потенциала межмолекулярного взаимодействия на структуру ударной волны. Полученные численные результаты сравнены с другими теоретическими результатами.

### 1. Introduction

THE INFLUENCE of the intermolecular potential on the structure and width of the shock wave has been investigated by several authors [1-3]. All of them used some approximate methods, because it is not possible to solve the full Boltzmann equation even for the case of the plane shock wave.

In this paper the analysis of intermolecular potential is based on approximate solutions obtained using Tamm's variational method [4]. Originally Tamm proposed this method assuming the hard spheres model of molecules.

In the more general case, when one allows the potential to be in the form  $u(r) = k/r^s$ , where  $k$  is constant, or in the form of the Lenard-Jones potential, the calculations of the collision integral are much more complicated than in the case of hard spheres. Thus as a starting point for further calculations and to check the method we assume that the gas is two-dimensional, i.e. that it has only two translational degrees of freedom, one parallel, and the second perpendicular to the direction of the gas flow.

Such a two-dimensional gas model has already been exploited by CHAHINE [5]; he used it for the analysis of a particular iteration scheme of solving the Boltzmann equation. E. G. D. Cohen analysing the generalized Boltzmann equation for the dense gas also considered the two-dimensional gas model [14, 15].

Tamm's variational method demands minimalization of the functional:

$$(1.1) \quad S = \int \int d\mathbf{v} dx [\mathbf{v} \text{grad} f - \chi(f, f)]^2,$$

where  $f$  is the distribution function,  $\mathbf{v}$  — the velocity vector,  $\chi(f, f)$  — the nonlinear collision term;  $\mathbf{v} = [v_x, v_y]$ .

Other variational methods were proposed by ROSEN [6], OBERAI [7], NARASIMHA [8], but Tamm's method seems to be the most straightforward one.

Tamm assumed that the distribution function has the form:

$$(1.2) \quad f = \frac{1-h(x)}{2} f_1(\mathbf{v}) + \frac{1+h(x)}{2} f_2(\mathbf{v})$$

(a similar form has been assumed by MOTT-SMITH [9]).

Here, for two-dimensional gas,

$$(1.3) \quad f_i(\mathbf{v}) = n_i \left( \frac{m_i}{2\pi k T_i} \right) \exp \left\{ -\frac{m_i}{2k T_i} [(v_x - u_i)^2 + v_y^2] \right\}, \quad i = 1, 2$$

are Maxwellian functions in minus and plus infinity, respectively (i.e. in front and behind the shock wave);  $T_i$  is the temperature,  $n_i$  the number density of molecules,  $\mathbf{u}_i = [u_i, 0]$  are the flow velocity vectors whose only non-vanishing component is in the  $x$ -direction.

The function  $h(x)$  minimizes the functional (1.1) and has the following properties:

$$(1.4) \quad \lim_{x \rightarrow \infty} h(x) = 1, \quad \lim_{x \rightarrow -\infty} h(x) = -1.$$

Assuming the form of the distribution function (1.2), an appropriate Euler equation can be explicitly solved:

$$(1.5) \quad h(x) = \text{th} \left( x \sqrt{\frac{C}{A}} \right),$$

where  $A$  is constant for the chosen shock wave (definition — (2.13)), and where  $C$  depends on the collision term (hence also on an intermolecular potential) and will be defined later — (2.15).

It should be noted that the form (1.5) coincides with the structure of the weak shock wave found in 1910 by TAYLOR [10].

Our aim is to calculate  $A$  and  $C$  for two-dimensional gas with different intermolecular forces.

Clearly, one cannot expect to obtain results coinciding with three-dimensional theories or with the experimental data. However, the qualitative behaviour should be (and is proved to be) the same as in the three-dimensional case.

The proposed method can be extended in two directions. First, by introducing the three-dimensional gas model, second, by using the two-dimensional model for the investigation of more general cases, say the shock wave in a gas mixture. Work in this second direction is now in progress.

## 2. The collision integral

To evaluate the collision integral  $\chi(f, f)$  entering the functional (1.1), one needs to know the mechanics of an individual collision. This is equivalent to the motion of a single particle with the reduced mass  $\mu = (m_1 \cdot m_2)/(m_1 + m_2)$  ( $m_1, m_2$  are the masses of colliding particles) moving in a spherically symmetric field with the potential  $U(r)$ .

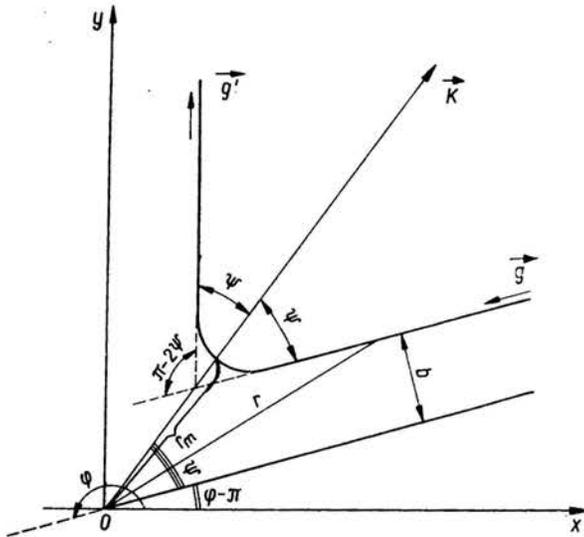


FIG. 1. One-body problem.

The resulting one-body problem is shown in Fig. 1. Using the conservation laws for energy and angular momentum, one gets the following expression:

$$(2.1) \quad \Psi = gb\mu \int_{r_{\min}}^{\infty} \frac{dr}{r \cdot \sqrt{2\mu r^2 \left[ \frac{1}{2} \mu g^2 - U(r) \right] - g^2 b^2 \mu^2}}.$$

Here  $b$  is the impact parameter, i.e. the distance of closest approach of particles in the absence of the  $U(r)$  potential;  $g$  is the initial (i.e. at time  $t = -\infty$ ) relative velocity vector of the colliding molecules.

From the conservation laws of momentum and energy for the colliding molecules, the relations between the velocity vectors of molecules before ( $\mathbf{v}, \mathbf{v}_1$ ) and after collision ( $\mathbf{v}', \mathbf{v}'_1$ ) are as follows:

$$(2.2) \quad \mathbf{v}' = \mathbf{v} - \mathbf{k} |g| \cos \Psi,$$

$$(2.3) \quad \mathbf{v}'_1 = \mathbf{g} + \mathbf{v} + \mathbf{k} |g| \cos \Psi,$$

where

$$(2.4) \quad \mathbf{g}' = \mathbf{v}'_1 - \mathbf{v}',$$

$$(2.5) \quad \mathbf{g} = \mathbf{v}_1 - \mathbf{v},$$

and

$$\mathbf{k} = [\cos(\Psi + \varphi - \pi), \sin(\Psi + \varphi - \pi)].$$

Clearly,

$$(2.6) \quad |g| = |g'| = g.$$

In the two-dimensional case the collision integral has the form

$$(2.7) \quad \chi(f, f) = 2 \int \{f, f\} g db d\mathbf{v}_1,$$

where

$$(2.8) \quad \{f, f\} = f(\mathbf{v}')f(\mathbf{v}'_1) - f(\mathbf{v})f(\mathbf{v}_1).$$

The use of (1.2) leads to the expression

$$(2.9) \quad \{f, f\} = \frac{1-h^2}{4} G(f_1, f_2),$$

where

$$(2.10) \quad G(f_1, f_2) = f_1(\mathbf{v}')f_2(\mathbf{v}'_1) - f_1(\mathbf{v})f_2(\mathbf{v}_1) + f_1(\mathbf{v}'_1)f_2(\mathbf{v}') - f_1(\mathbf{v}_1)f_2(\mathbf{v}).$$

The integral

$$(2.11) \quad H(\mathbf{v}) = 2 \int G(f_1, f_2) g db d\mathbf{v}_1$$

plays an important role in the theory because the functional  $S$  can be rewritten in the form

$$(2.12) \quad S = \int dx [Ah'^2 - 2(1-h^2)h'B + (1-h^2)^2C]$$

with the constants  $A, B, C$  determined as follows:

$$(2.13) \quad A = \int \frac{v^2}{4} (f_2 - f_1) d\mathbf{v},$$

$$(2.14) \quad B = \frac{1}{8} \int v_x (f_2 - f_1) H(\mathbf{v}) d\mathbf{v},$$

$$(2.15) \quad C = \frac{1}{16} \int H^2(\mathbf{v}) d\mathbf{v}.$$

The variation of  $S$ , i.e.

$$(2.16) \quad \delta S = \int dx \{2\delta h' [Ah' - (1-h^2)B] + 4\delta h [hh'B - C(1-h^2)h]\},$$

where  $h' = h_{,x}$  leads to the solution (1.5) mentioned above.

### Two-dimensional gas

In the two-dimensional case one can obtain all gas characteristics exactly in the same way as one does in the three-dimensional case.

The mean velocity is

$$(3.1) \quad \bar{v}^2 = \int d\mathbf{v} |\mathbf{v}| f(\mathbf{v}, t) = \frac{m}{2\pi kT} \int_0^{2\pi} \int_0^\infty \exp\left(-\frac{mv^2}{2kT}\right) v \cdot v dv d\varphi$$

$$= \sqrt{\frac{\pi kT}{2m}}, \quad v = |\mathbf{v}|$$

(where, in equilibrium  $f(\mathbf{v}, t) = f(\mathbf{v})$  and is the Maxwellian distribution function) instead of  $\sqrt{\frac{8kT}{m\pi}}$  what one gets for three-dimensional gas.

For further use we must introduce the mean free path  $l$ . The mean free path has an exact meaning only for hard spheres and thus we introduce it for this case (again in full accordance with the three-dimensional case)

$$(3.2) \quad l^{(2)} = \frac{\bar{v}^{(2)}}{\nu^{(2)}} = \frac{\int d\mathbf{v} |\mathbf{v}| f(\mathbf{v}, t)}{n^{(2)} 2\sigma \int d\mathbf{v} \int d\mathbf{v}_1 f(\mathbf{v}, t) f(\mathbf{v}_1, t) |\mathbf{v} - \mathbf{v}_1|}$$

Here  $\nu$  denotes the collision frequency ( $\nu^{(2)}$  for two-dimensional gas,  $\nu^{(3)}$  for three-dimensional gas),  $\sigma$  is the diameter of the rigid sphere (molecule),  $n$  denotes the number density (respectively:  $n^{(2)}$  for two-dimensional gas,  $n^{(3)}$  for three-dimensional gas) and  $l$  is the mean molecular free path (respectively:  $l^{(2)}$  for two-dimensional gas,  $l^{(3)}$  for three-dimensional gas). The only difference from the three-dimensional case is that  $2\sigma$  appears here instead of  $\pi\sigma^2$  in the denominator. Introducing the velocity vector of the center of mass

$$(3.3) \quad \mathbf{w} = \frac{1}{2} (\mathbf{v}_1 + \mathbf{v}),$$

we can write

$$(3.4) \quad \mathbf{v} = \mathbf{w} - \frac{1}{2} \mathbf{g},$$

$$(3.5) \quad \mathbf{v}_1 = \mathbf{w} + \frac{1}{2} \mathbf{g}$$

and thus the collision frequency for two-dimensional gas is

$$(3.6) \quad \nu^{(2)} = 2\sigma n^{(2)} \int d\mathbf{v} \int d\mathbf{v}_1 f(\mathbf{v}, t) f(\mathbf{v}_1, t) g = \sigma 2\sqrt{2} \sqrt{\frac{kT\pi}{2m}} n^{(2)} = 2\sqrt{2} \bar{v}^{(2)} n^{(2)} \sigma.$$

For three-dimensional gas the collision frequency is

$$(3.7) \quad \nu^{(3)} = 4\pi \sqrt{\frac{kT}{m\pi}} n^{(3)} \sigma^2.$$

Finally, for two-dimensional gas

$$(3.8) \quad l^{(2)} = \frac{1}{2\sqrt{2} n^{(2)} \sigma}$$

instead of

$$(3.8') \quad l^{(3)} = \frac{1}{\sqrt{2} n^{(3)} \pi \sigma^2}$$

for the three-dimensional one.

One should note that the number densities in these formulae have different meaning and dimensions. The mean free path for the gas model different from the hard spheres

model is defined by Eq. (3.2) putting instead of  $\sigma$  some type of effective diameter  $\tilde{\sigma}$ . In all cases, however, we use non-dimensional magnitudes and  $\tilde{\sigma}$  as the unit of length.

The non-dimensional mean free-path is

$$(3.9) \quad l^{*(2)} = \frac{l^{(2)}}{\tilde{\sigma}} = \frac{1}{2\sqrt{2}n^*}$$

and, accordingly,

$$(3.10) \quad l^{*(3)} = \frac{l^{(3)}}{\tilde{\sigma}} = \frac{1}{\pi\sqrt{2}n^*}.$$

In the formulae (3.9) and (3.10)  $n^*$  is the non-dimensional number density of molecules:

$$(3.11) \quad n^* = n^{(3)}\sigma^3 = n^{(2)}\sigma^2 = \frac{p^*}{T^*}.$$

The last equality follows from the assumption that both, the two-dimensional and three-dimensional gases, are ideal;  $p^*$ ,  $T^*$  are non-dimensional pressure and temperature.

From Eqs. (3.9) and (3.10) it follows that

$$(3.12) \quad \frac{l^{*(2)}}{l^{*(3)}} = \frac{\pi}{2}.$$

#### 4. The numerical procedure

The resulting expression (1.5) contains two numbers  $A$  and  $C$ .  $A$  can be found analytically but  $C$  must be found using either some series expression (as in [4]) or numerical procedure.

For two-dimensional gas  $C$  is the four-fold integral over infinite velocity space.

Due to these boundaries it was necessary to introduce an appropriate correction.

Let  $F = F(f_1, f_2)$  be the function similar to the  $H(\mathbf{v})$  function (2.11), i.e. such that it is a function of combination of the products of  $f_1$  and  $f_2$ .

This form suggests the type of correction which has been used, namely:

$$(4.1) \quad \int_{-\infty}^{\infty} F d\mathbf{v} = d_1(\alpha, \delta) d_2(\alpha, \delta) \int_{\alpha}^{\delta} F d\mathbf{v}.$$

The correction factors  $d_1(\alpha, \delta)$ ,  $d_2(\alpha, \delta)$  are defined by the formulae

$$(4.2) \quad d_1(\alpha, \delta) = \frac{\int_{-\infty}^{\infty} f_1 d\mathbf{v}}{\int_{\alpha}^{\delta} f_1 d\mathbf{v}} = \frac{n_1}{\int_{\alpha}^{\delta} f_1 d\mathbf{v}}$$

and

$$(4.3) \quad d_2(\alpha, \delta) = \frac{\int_{-\infty}^{\infty} f_2 d\mathbf{v}}{\int_{\alpha}^{\delta} f_2 d\mathbf{v}} = \frac{n_2}{\int_{\alpha}^{\delta} f_2 d\mathbf{v}}.$$

The correction factors  $d_1, d_2$  or, strictly speaking,  $|d_1 - 1|, |d_2 - 1|$  can be treated as the measures of the accuracy of the calculations. We assumed these values do not exceed  $10^{-3}$ , and appropriately we chose the step of the integration.

Our computations run as follows:

1. In the front of the shock wave we assume  $n_1^* = 1, T_1^* = 1$  (where  $n^* = n^{(2)}\sigma^2, T^* = \frac{k}{\varepsilon} T, k$  being the Boltzmann constant,  $\varepsilon/k$  — the so-called potential parameter); the only free parameter was thus the Mach number  $M_1$  (or  $u_1^*$ ). For two-dimensional gas  $\gamma = c_p/c_v = 2$  [11], where  $c_p, c_v$  are the specific heats.
2. The values of  $n_2^*, T_2^*, u_2^*$  are obtained from the Hugoniot's conditions.
3. The  $A^*$  integral can be directly found and it is equal to

$$(4.4) \quad A^* = A\sigma^4 = \frac{(-1)}{4\pi} n_1^* n_2^* \frac{1}{T_1^* T_2^* \left(\frac{1}{T_1^*} + \frac{1}{T_2^*}\right)^2} \left[ 1 + 4 \frac{\left(\frac{u_1^*}{T_1^*} + \frac{u_2^*}{T_2^*}\right)^2}{\frac{1}{T_1^*} + \frac{1}{T_2^*}} \right] \times \exp \left\{ 2 \left[ -\frac{u_1^{*2}}{T_1^*} - \frac{u_2^{*2}}{T_2^*} + \frac{\left(\frac{u_1^*}{T_1^*} + \frac{u_2^*}{T_2^*}\right)^2}{\frac{1}{T_1^*} + \frac{1}{T_2^*}} \right] \right\} + \frac{1}{32\pi} \sum_{i=1}^2 n_i^{*2} \left( 1 + 8 \frac{u_i^{*2}}{T_i} \right).$$

4. To calculate the angle  $\Psi$  (2.1) we change the variable and we get

$$(4.5) \quad \Psi = \int_0^{\beta_0} \frac{d\beta}{\sqrt{1 - \beta^2 - U^*/g^{*2}}},$$

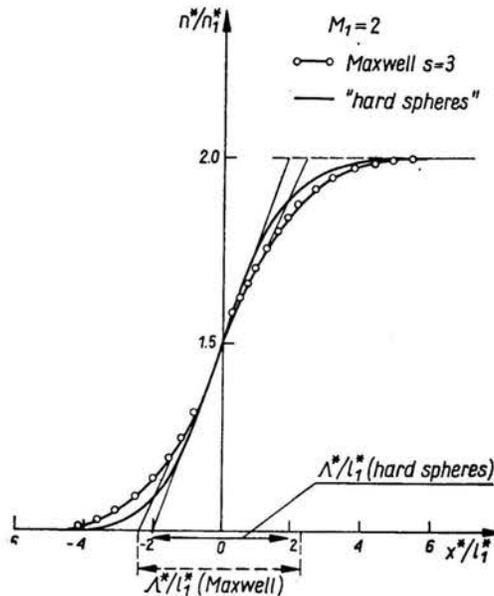


FIG. 2. The influence of the intermolecular potential on the shock wave structure ( $M_1 = 2$ ).

where

$$\beta = \frac{b}{r} = \frac{b^*}{r^*}.$$

Here  $\beta_0$  is the root of the functional equation

$$(4.6) \quad 1 - \beta^2 - \frac{U^*(\beta)}{g^{*2}} = 0,$$

where  $U^*(\beta) = U/\varepsilon$  is the non-dimensionalized potential and  $g^{*2} = \frac{1}{2} \frac{\mu}{\varepsilon} g^2$  ( $g$  is defined in Eq. (2.5)).

5. The subintegral function  $G$  (see Eq. (2.10)) depends on  $v$ ,  $v_1$  and  $v'_1$ ,  $v'$ , which in turn depend on  $\Psi$ .

The most time-consuming procedure is the calculation of the integral  $C^* = C \cdot \sigma^6$ ,  $C$  being determined by Eq. (2.15).

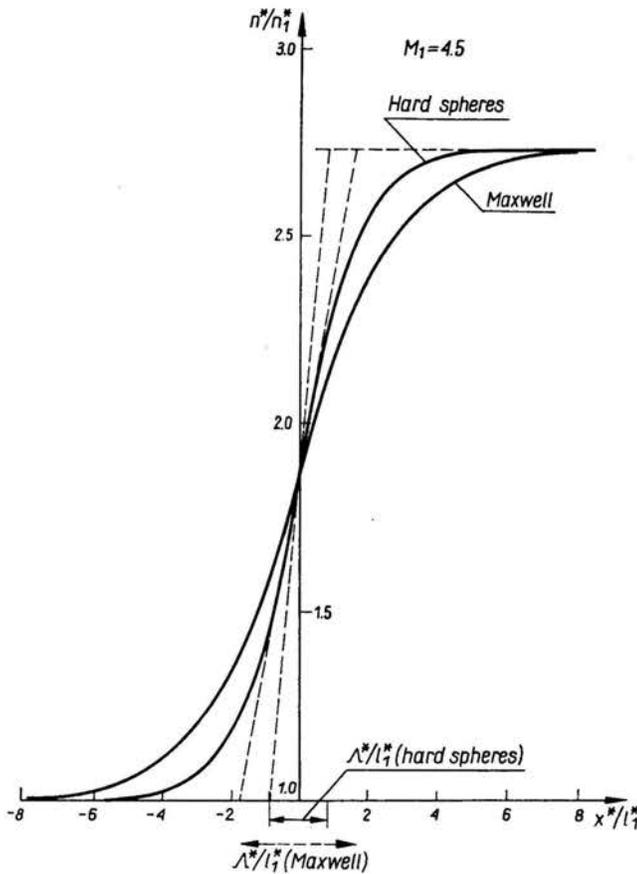


FIG. 3. The influence of the intermolecular potential on the shock wave structure ( $M_1 = 4.5$ ).

The non-dimensional width of the shock wave is equal to

$$(4.7) \quad \Lambda^* = \frac{\Lambda}{\sigma} = \frac{A^*}{C^*}.$$

6. Using Eq. (1.2) we find the distribution function in any desired point in the flow.

## 5. Results and conclusions

The influence of the intermolecular potential for Mach numbers 2 and 4.5 on density profiles is shown in Figs. 2 and 3.

As in the three-dimensional case there are two limiting cases, namely hard spheres molecules, what corresponds to  $s = \infty$  in the formula  $U(r) = K/r^s$ , and Maxwellian molecules, what in two-dimensions corresponds to  $s = 3$  [5, 12, 13].

For  $3 < s < \infty$  the shock structure lies between these shock structures for two limits. All magnitudes are related to the conditions before the shock (denoted by the subscript 1). The pressure and temperature profiles have a similar form. The main characteristic of the shock wave is its non-dimensional thickness  $\Lambda^*/l_1^*$  which is equal to  $\frac{1}{l_1^*} \sqrt{C^*/A^*}$  ( $l_1^*$  denotes the non-dimensional mean free path for the gas in front of the shock wave).

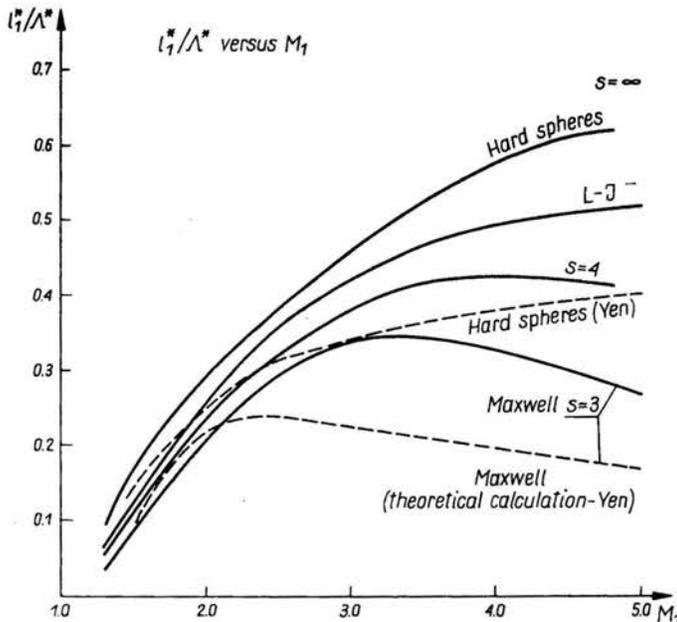


FIG. 4. The inverse of the shock wave thickness versus Mach number  $M_1$ .

In Fig. 4 the inverse of the shock wave thickness versus Mach number  $M_1$  for different intermolecular potentials is shown. The asymptotic value for the infinitely strong shock wave found by Tamm is equal to  $\frac{l_1^*}{\Lambda^*} = \frac{1}{0.503} = 1.988$  and is much higher than

the values shown in Fig. 4 for  $M < 5$ . For the weak shock wave the inverse of its thickness tends to zero. The distribution function for the hard spheres is presented in Figs. 5 and 6. At the center of the shock wave this function has a usual bell-shape form with respect to the  $v_y^*$  axis.

The form of  $f$  across the shock (i.e. along the  $x$  axis) for  $v_y = 0$  is presented in Fig. 6.

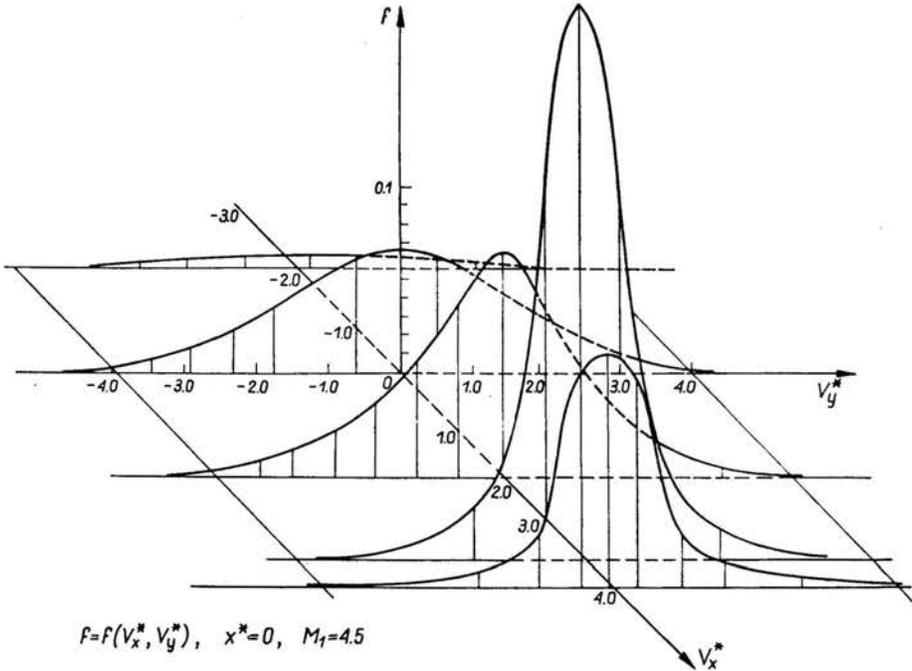


FIG. 5. The distribution function versus  $v_x^*, v_y^*$  ( $M_1 = 4.5, x^* = 0$ ).

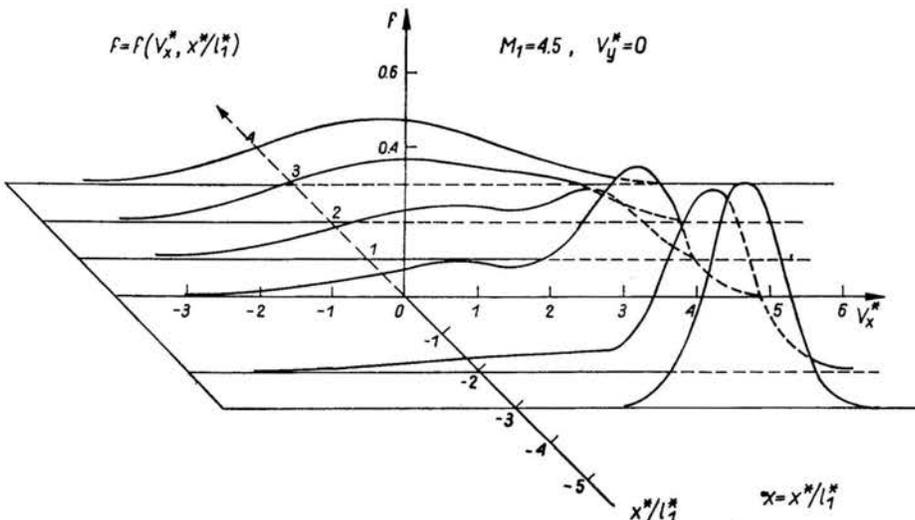


FIG. 6. The distribution function versus  $v_x^*, x^*/l_1^*$  ( $M_1 = 4.5$ ).

For  $x = \pm 3$  the distribution function does not differ significantly from the one assumed at  $\pm \infty$ .

At the middle  $f$  has two maxima, and clearly this results from our initial assumption (1.2) concerning the form of the distribution function.

Finally, we should mention that the results presented in Fig. 4 are in qualitative agreement with those obtained for the three-dimensional case [1, 2, 3], but are shifted:  $I^{(2)}/A^{(2)}$  is greater than  $I^{(3)}/A^{(3)}$ . For the hard spheres model, Maxwellian molecules and  $s^{(2)} = 4$  (i.e.  $s^{(3)} = 5$ ) the comparison is given in Fig. 4.

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POLISH ACADEMY OF SCIENCES  
INSTITUTE OF FUNDAMENTAL TECHNOLOGICAL RESEARCH.

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