Derivation of Hydrodynamic Equations for the Quantum Systems of Diatomic Molecules

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Bogolyubov's method of derivation of the hydrodynamic equations from a quantum-statistical formalism, based on the array of distribution operators for clusters of s molecules, is adapted to the derivation of the hydrodynamic equations for a fluid composed of diatomic molecules. The general form of the hydrodynamic equations with an additional equation of angular momentum, which is coupled with the momentum equation through the antisymmetric part of the stress tensor, is obtained and all the interesting hydrodynamic quantities are calculated. A general procedure of derivation of the hydrodynamic equations by successive approximations is proposed and the equations of zeroth approximation are discussed.

INTRODUCTION

THE purpose of this paper is to derive hydrodynamic equations, taking into account the internal structure of diatomic molecules. From the macroscopic point of view the hydrodynamic variables describing the state of a diatomic fluid at any point of space and any time are: density $g(x_l,t)$, velocity $u_k(x_l,t)$, intrinsic energy $\epsilon(x_l,t)$, and the additional macroscopic variable called the angular velocity of the fluid at given point of space and time, $\omega_k(x_l,t)$. This latter quantity is coupled by means of the inertia density tensor of the fluid at a given point and time with the intrinsic angular momentum of the fluid:

$$g(x_l,t)m_k(x_l,t)=i_{kn}(x_l,t)\omega_n(x_l,t).$$

The phenomenological equations of motion of hydrodynamic variables given above follow easily from the principles of conservation of mass, momentum, angular momentum and energy. They are:

Principle of conservation of mass

$$\frac{D}{Dt}\int_V gd_{(3)}v=0$$

Principle of conservation of momentum

$$\frac{D}{Dt}\int_V gu_k d_{(3)}v=\int_F T_{kl}df_l$$

Principle of conservation of angular momentum

$$\frac{D}{Dt}\int_V g(\epsilon_{kij}x_iu_j+m_k)d_{(3)}v=\int_F (\epsilon_{kij}x_iT_{jl}+Q_{kl})df_l$$

Principle of conservation of energy

$$\frac{D}{Dt}\int_V g(\tfrac{1}{2}u^2+\tfrac{1}{2}m_l\omega_l+\epsilon)d_{(3)}v=\int_F (u_iT_{il}+\omega_iQ_{il}+q_l)df_l$$

Equation of continuity

$$\frac{Dg}{Dt}+gu_{k,k}=0$$

Equation of momentum

$$g\frac{Du_k}{Dt}=T_{kl,l}$$

Equation of angular momentum

$$g\frac{Dm_k}{Dt}=Q_{kl,l}-\epsilon_{kij}T_{ij}$$

Equation of energy

$$g\frac{D}{Dt}(\epsilon+\tfrac{1}{2}m_l\omega_l)=u_{i,l}T_{il}+(\omega_iQ_{il}+q_l)_{,l}$$

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where T_{kl} is the stress tensor (in the usual sense), Q_{kl} is the stress tensor of couples, and q_k is the heat flow vector.

In order to complete the phenomenological hydrodynamic equations, the relations between T_{kl}, Q_{kl}, and q_k and the hydrodynamic variables must be given. Various forms of these relations distinguish various media. However, the full phenomenological theory of these relations is not known as yet. In the past years Grad[1] has given one of the possible proposals for the above-mentioned relations, based on the thermodynamics of irreversible processes. Naturally, it would be very desirable—both for the practical importance of the hydrodynamic equations for diatomic fluids and gases (e.g., air) and for the methodological role—to derive the relations between the quantities T_{kl}, Q_{kl}, q_k, and the hydrodynamic variables from the microscopic assumptions by means of a statistical formalism. The first such approach, for gases composed of rough spheres, was done by Bryan, Pidduck, and Jeans. One of the latest papers about this problem is the work by Curtiss.[2] All these works are based on the Boltzmann equation, that is on the kinetic theory of gases, and give no information about the antisymmetric part of the stress tensor. Therefore they give equations in which there is no coupling between the equation of momentum and the equation of angular momentum.

The task of this paper is to derive the general form of hydrodynamic equations for diatomic fluids by means of the formalism of quantum statistics, which is not related with the Boltzmann equation. For this purpose the Bogolyubov method of an array of distribution operators[3-7] has been adapted and generalized for diatomic fluids. In this connection the equations of motion for the distribution operators of clusters of s diatomic molecules have been derived, the operators of mass density, momentum, angular momentum, and energy of the fluid at given point of space have been introduced, their average values have been calculated, and afterwards the equations, describing the evolution of these values in time, have been found. They are the equations which are the macroscopic hydrodynamic equations. In this manner the quantities T_{kl}, Q_{kl}, q_k are represented by means of matrix elements of distribution operators for one and two molecules f_1 and f_2, respectively. The parts of T_{kl}, Q_{kl}, q_k connected with the f_1 function are named the kinetic parts and those

connected with f_2 and depending on the intermolecular influence (which is assumed noncentral) are named the dynamic parts of these quantities. After finding the general form of the hydrodynamic equations, a general scheme of finding distribution operators is proposed, which is an adaptation of Bogolyubov's method for monatomic fluids. Certain peculiarities of this method, which appear for diatomic fluids and which complicate the problem to a great extent, are discussed. The system of equations for the expansion coefficients of f_s matrix elements is so difficult that it has not been solved until now even for the case of monatomic fluids. For this reason the problem has been limited to the qualitative discussion of the equations in the zeroth approximation. They correspond to the Euler equations for monatomic fluids. In particular, it has been shown that the stress tensor has no symmetry properties and this fact gives the coupling between the equation of momentum and that of angular momentum, even in the equations of zeroth approximation. Naturally the special case, that some peculiar form of the expansion coefficients of the f_s functions may cause the vanishing of this coupling, is not excluded entirely. No doubt further investigations will shed more light on this problem.

A similar program based however on classical statistics was already published by the author.[8]

1. DISTRIBUTION OPERATORS AND THEIR EQUATIONS OF MOTION

Let us assume that N diatomic molecules are present in a certain volume V. The Hamiltonian of this system may be written in the form

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\{\Delta_{i1}+\Delta_{i2}+U_i(r_k^{(i1)},r_k^{(i2)})\}$$
$$+\sum_{i\leq j}^{N}\phi_{ij}(r_k^{(i1)},r_k^{(i2)},r_k^{(j1)},r_k^{(j2)}), \quad (1.1)$$

where $r_k^{(i1)}$ describes the position of the first atom of the ith molecule and $r_k^{(i2)}$ gives the position of the second atom of the ith molecule. ϕ_{ij} is the interaction potential between the ith and the jth molecule (an intermolecular potential), and in the case $i=j$ it is an intramolecular potential. U_i represents interaction potential of the ith molecule with the wall of a vessel, which in our system must be present since the fluid stays in a fixed volume V.

A complete description of the state of system should give the density operator ρ, defined by its equation of motion $\partial\rho/\partial t=[H,\rho]=(H\rho-\rho H)/i\hbar$ with the normalization condition $\mathrm{Sp}\rho=1$ and by the specification of the kind of statistics. In our case we assume that the molecules are subject to the Bose statistics, i.e., we require that $P\rho=\rho P=\rho$, where P is the permutation

[1] H. Grad, Comm. Pure Appl. Math. **5**, 455 (1952).

[2] C. F. Curtiss, J. Chem. Phys. **24**, 225 (1956).

[3] N. N. Bogolyubov, *The Problems of Dynamical Theory in the Statistical Physics* (in Russian) (Moscow, 1946).

[4] N. N. Bogolyubov, *Collection of Works of Mathematical Institute of U.S.S.R. Academy of Sciences* (in Ukrainian) No. 10, 41 (1948).

[5] N. N. Bogolyubov, *Lectures on the Quantum Statistics* (in Ukrainian) (Kiyov, 1949).

[6] K. P. Gurov, J. Exptl. Theoret. Phys. (U.S.S.R.) **18**, 110 (1948).

[7] K. P. Gurov, J. Exptl. Theoret. Phys. (U.S.S.R.) **20**, 279 (1950).

[8] R. Želazny, Bull. acad. polon. sci. Classe III, **6**, 203 (1958).

operator. The average value of any dynamical variable Z may be calculated by means of density operator according to the formula $\bar{Z} = \mathrm{Sp} Z\rho$. However, as it is impossible to find an explicit form of a density operator (N is a very great number), following Bogolyubov[3-5] and Born and Green[9] we introduce the distribution operators for one, two, $\cdots$, s molecules according to the formula

$$F_s = \Omega_V^s \mathop{\mathrm{Sp}}_{(s+1,\cdots,N)} \rho,$$

where Ω_V is the volume of the configurational space of diatomic molecules, corresponding to the real volume V of the system.

Using these operators, the average values of any dynamical variable of the form

$$Z = \sum_{1 \le j_1 \le \cdots \le j_s \le N} A(j_1, j_2, \cdots, j_s)$$

can be calculated according to the formula

$$\bar{Z} = \binom{N}{s} \Omega_V^s \,\mathrm{Sp} A F_s.$$

Acting with the operator "Sp" on the equation of motion of the density operator and multiplying by Ω_V^s, the equations of motion for the F_s operators are easily available, namely

$$\frac{\partial F_s}{\partial t} = [H_s, F_s] + \frac{N}{\Omega_V}\left(1 - \frac{s}{N}\right)$$

$$\times \mathop{\mathrm{Sp}}_{(s+1)} \left[\sum_{i=1}^{s} \phi_{i,\,s+1}, F_{s+1}\right] + \left[\sum_{i=1}^{s} U_i, F_s\right],$$

where H_s denotes the Hamiltonian of a cluster consisting of s molecules.

We shall now consider the asymptotic case, characterized by the expansion of the domain V into the whole space (the influence of the walls of any vessel will now be neglected) and by the increase of the number N to ∞, such that $\Omega_V/N = \omega = \text{const}$. This passage to the asymptotic problem is characteristic of the kinetic theory of fluids, even in such cases, in which is explicitly not formulated. In the asymptotic case some of our previous formulas are changed into the following forms:

$$F_s = \lim_{V \to \infty, N \to \infty} \Omega_V^s \mathop{\mathrm{Sp}}_{(s+1,\cdots,N)} \rho; \quad \bar{Z} = \frac{1}{s!\,\omega^s} \mathrm{Sp} A F_s, \quad (1.2)$$

$$\frac{\partial F_s}{\partial t} = [H_s, F_s] + \frac{1}{\omega} \mathop{\mathrm{Sp}}_{(s+1)} \left[\sum_{i=1}^{s} \phi_{i,\,s+1}, F_{s+1}\right]. \quad (1.3)$$

The operators F_s thus defined have the following

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[9] M. Born and H. S. Green, Proc. Roy. Soc. (London) **A188**, 10 (1946).

properties:

(1) They are Hermitian operators.
(2) They are normalized in the following manner:

$$F_s = \lim_{V \to \infty, N \to \infty} \frac{1}{\Omega_V} \mathop{\mathrm{Sp}}_{(s+1)} F_{s+1}, \quad \lim_{V \to \infty, N \to \infty} \frac{1}{\Omega_V} \mathrm{Sp} F_1 = 1.$$

(3) They are invariant under the action of permutation operator.

Moreover, the F_s operators must comply with the condition of "decreased correlation," expressing the fact that when the distances between s molecules tend to infinity, the F_s operators tend to s times the corresponding F_1 operators.

Let us distinguish one state from all the other possible states of our system and call it the spatially uniform state. This state is defined as the state in which the F_s operator matrices, in a coordinate representation, will be invariant under the influence of a translation of the coordinate system

$$\langle r_k'^{(11)} + r_k^{(0)}, r_k'^{(12)} + r_k^{(0)}, \cdots, r_k'^{(s1)} + r_k^{(0)},$$
$$r_k'^{(s2)} + r_k^{(0)} | F_s | r_k''^{(11)} + r_k^{(0)}, r_k''^{(12)} + r_k^{(0)}, \cdots,$$
$$r_k''^{(s1)} + r_k^{(0)}, r_k''^{(s2)} + r_k^{(0)}\rangle \equiv \langle r_k'^{(11)}, r_k'^{(12)}, \cdots,$$
$$r_k'^{(s1)}, r_k'^{(s2)} | F_s | r_k''^{(11)}, r_k''^{(12)}, \cdots, r_k''^{(s1)}, r_k''^{(s2)}\rangle.$$

By performing the coordinate transformation

$$r_k^{(i)} = r_k^{(i1)} - r_k^{(i2)}, \quad R_k^{(i)} = \tfrac{1}{2}(r_k^{(i1)} + r_k^{(i2)}),$$

we divide the variables into two groups; one of them is invariant under the translation, and the second one is covariant under the translation of the coordinate system. These new variables can be so transformed that only one of the four vector variables of the F_1 operator matrix will be covariant under the coordinate translation:

$$\langle r_k'^{(1)}, R_k'^{(1)} | F_1 | r_k''^{(1)}, R_k''^{(1)}\rangle = f_1[\tfrac{1}{2}(R_k'^{(1)} + R_k''^{(1)}),$$
$$\tfrac{1}{2}(r_k'^{(1)} + r_k''^{(1)}), R_k'^{(1)} - R_k''^{(1)}, r_k'^{(1)} - r_k''^{(1)}]$$
$$= f_1(\xi_k^{(1)}, \rho_k^{(1)}, \eta_k^{(1)}, \sigma_k^{(1)}).$$

Among the arguments $\xi_k^{(1)}, \rho_k^{(1)}, \eta_k^{(1)}, \sigma_k^{(1)}$ the first one, i.e., $\xi_k^{(1)}$ is covariant under the coordinate translation. Similarly in the matrices of F_s operators we may also distinguish only one vector variable, namely $\xi_k^{(1)}$ which is covariant under the coordinate translation:

$$\langle r_k'^{(1)}, R_k'^{(1)}, \cdots, r_k'^{(s)}, R_k'^{(s)} | F_s | r_k''^{(1)}, R_k''^{(1)}, \cdots,$$
$$r_k''^{(s)}, R_k''^{(s)}\rangle = f_s[\tfrac{1}{2}(R_k'^{(1)} + R_k''^{(1)}),$$
$$\tfrac{1}{2}(r_k'^{(1)} + r_k''^{(1)}), R_k'^{(1)} - R_k''^{(1)}, r_k'^{(1)} - r_k''^{(1)},$$
$$\tfrac{1}{2}(R_k'^{(2)} + R_k''^{(2)} - R_k'^{(1)} - R_k''^{(1)}), \tfrac{1}{2}(r_k'^{(2)} + r_k''^{(2)}),$$
$$R_k'^{(2)} - R_k''^{(2)}, r_k'^{(2)} - r_k''^{(2)}, \cdots,$$
$$\tfrac{1}{2}(R_k'^{(s)} + R_k''^{(s)} - R_k'^{(1)} - R_k''^{(1)}), \tfrac{1}{2}(r_k'^{(s)} + r_k''^{(s)}),$$
$$R_k'^{(s)} - R_k''^{(s)}, r_k'^{(s)} - r_k''^{(s)}] = f_s(\xi_k^{(1)}, \rho_k^{(1)}, \eta_k^{(1)},$$
$$\sigma_k^{(1)}, \xi_k^{(2)}, \rho_k^{(2)}, \eta_k^{(2)}, \sigma_k^{(2)}, \cdots, \xi_k^{(s)}, \rho_k^{(s)}, \eta_k^{(s)}, \sigma_k^{(s)})$$

The suitable transformation is apparent from the

formula given above. According to this transformation, the equations of motion of the F_s operators in the coordinate representation have been transformed, namely

$$\frac{\partial f_s}{\partial t} = \frac{2i\hbar}{m}\left[\sum_{i=1}^{s}\frac{\partial^2 f_s}{\partial\rho_k^{(i)}\partial\sigma_k^{(i)}} + \frac{1}{4}\frac{\partial^2 f_s}{\partial\xi_k^{(1)}\partial\eta_k^{(1)}} - \frac{1}{4}\sum_{i=2}^{s}\left(\frac{\partial^2 f_s}{\partial\eta_k^{(1)}\partial\xi_k^{(i)}} - \frac{\partial^2 f_s}{\partial\eta_k^{(i)}\partial\xi_k^{(i)}}\right)\right]$$

$$+\frac{1}{i\hbar}\sum_{i\leqslant j}^{s}(\phi_{i'j'}-\phi_{i''j''})f_s + \frac{1}{\omega i\hbar}\sum_{i=1}^{s}\int\left|(\phi_{i',(s+1)''}-\phi_{i'',(s+1)''})f_{s+1}\right|_{\eta_k^{(s+1)}=\sigma_k^{(s+1)}=0}d_{(3)}\xi^{(s+1)}d_{(3)}\rho^{(s+1)}, \quad (1.4)$$

where by $\phi_{i'j'}$ and $\phi_{i''j''}$ we understand $\langle r_k'^{(i)}, R_k'^{(i)}, r_k'^{(j)}, R_k'^{(j)}|\phi_{ij}|r_k'^{(i)}, R_k'^{(i)}, r_k'^{(j)}, R_k'^{(j)}\rangle$ and $\langle r_k''^{(i)}, R_k''^{(i)}, r_k''^{(j)}, R_k''^{(j)}|\phi_{ij}|r_k''^{(i)}, R_k''^{(i)}, r_k''^{(j)}, R_k''^{(j)}\rangle$ expressed by $\xi_k^{(1)}, \xi_k^{(i)}, \rho_k^{(i)}, \eta_k^{(i)}, \sigma_k^{(i)}, \xi_k^{(j)}, \rho_k^{(j)}, \eta_k^{(j)}, \sigma_k^{(j)}$ according to the transformation formulas. By $\phi_{i',(s+1)''}$ and $\phi_{i'',(s+1)''}$ we understand $\langle r_k'^{(i)}, R_k'^{(i)}, r_k''^{(s+1)}, R_k''^{(s+1)}|\phi_{i,s+1}|r_k'^{(i)}, R_k'^{(i)}, r_k''^{(s+1)}, R_k''^{(s+1)}\rangle$ and $\langle r_k''^{(i)}, R_k''^{(i)}, r_k''^{(s+1)}, R_k''^{(s+1)}|\phi_{i,s+1}|r_k''^{(i)}, R_k''^{(i)}, r_k''^{(s+1)}, R_k''^{(s+1)}\rangle$ with exchange of arguments as discussed above.

2. OPERATORS OF HYDRODYNAMIC VARIABLES AND THEIR AVERAGE VALUES

For the computation of observables which are interesting from the hydrodynamic point of view, the following operators are introduced:

the density operator at the point x_s,

$$G(x_s) = m\sum_{i=1}^{N}\{\delta_{(3)}(R_s^{(i)}-x_s)+\delta_{(3)}(R_s^{(i)}-x_s)\}; \quad (2.1)$$

the momentum operator at the point x_s,

$$I_l(x_s) = -\frac{i\hbar}{2}\sum_{i=1}^{N}\left\{\frac{\partial}{\partial R_l^{(i)}}\delta_{(3)}(R_s^{(i)}-x_s)+\delta_{(3)}(R_s^{(i)}-x_s)\frac{\partial}{\partial R_l^{(i)}}\right\}; \quad (2.2)$$

the angular momentum operator at the point x_s,

$$M_l(x_s) = -\frac{i\hbar}{2}\sum_{i=1}^{N}\left\{\sum_{j=1}^{2}\left[\epsilon_{lmn}r_m^{(ij)}\frac{\partial}{\partial r_n^{(ij)}}\delta_{(3)}(R_s^{(i)}-x_s)+\delta_{(3)}(R_s^{(i)}-x_s)\epsilon_{lmn}r_m^{(ij)}\frac{\partial}{\partial r_n^{(ij)}}\right]\right\}; \quad (2.3)$$

the energy operator at the point x_s,

$$E(x_s) = \frac{1}{2}\sum_{i=1}^{N}\{T_i\delta_{(3)}(R_s^{(i)}-x_s)+\delta_{(3)}(R_s^{(i)}-x_s)T_i$$
$$+\phi_{ii}\delta_{(3)}(R_s^{(i)}-x_s)+\delta_{(3)}(R_s^{(i)}-x_s)\phi_{ii}\}$$
$$+\frac{1}{2}\sum_{i<j}^{N}\{\phi_{ij}\delta_{(3)}(R_s^{(i)}-x_s)$$
$$+\delta_{(3)}(R_s^{(i)}-x_s)\phi_{ij}\}; \quad (2.4)$$

where T_i denotes the kinetic energy operator of the ith molecule. Average values of these operators are:

$$\bar{G}(x_s,t) = \frac{2m}{\omega}\int f_1(x_s,\rho_s^{(1)},0,0)d_{(3)}\rho^{(1)} \equiv \frac{2m}{\omega}\int[f_1]d_{(3)}\rho^{(1)}, \quad (2.5)$$

$$\bar{I}_l(x_s,t) = -\frac{i\hbar}{\omega}\int\left[\frac{\partial f_1}{\partial\eta_l^{(1)}}\right]d_{(3)}\rho^{(1)}, \quad (2.6)$$

$$\bar{M}_l(x_s,t) = \epsilon_{lmn}x_m\bar{I}_n(x_s,t) - \frac{i\hbar}{\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial f_1}{\partial\sigma_n^{(1)}}\right]d_{(3)}\rho^{(1)}, \quad (2.7)$$

$$\bar{E}(x_s,t) = -\frac{\hbar^2}{m\omega}\int\left[\frac{\partial^2 f_1}{\partial\sigma_k^{(1)}\partial\sigma_k^{(1)}}+\frac{1}{4}\frac{\partial^2 f_1}{\partial\eta_k^{(1)}\partial\eta_k^{(1)}}+\frac{1}{16}\frac{\partial^2 f_1}{\partial\xi_k^{(1)}\partial\xi_k^{(1)}}\right]d_{(3)}\rho^{(1)}$$

$$+\frac{1}{\omega}\int[\phi_{1'1'}f_1]d_{(3)}\rho^{(1)}+\frac{1}{2\omega^2}\int[\phi_{1'2'}f_2]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (2.8)$$

where the meaning of [ ] is clear from the first formula. For the spatially uniform state all average values given above (without the external part of angular momentum) do not depend on the x_s, since the f_1 and f_2 functions do not depend on the $\xi_k^{(1)}$, in place of which one should put x^s. It follows that if a spatially uniform state is also independent of the time, it is a state in which our system has a constant density, momentum, intrinsic angular momentum [the second term in the formula (2.7)], and energy at any point of the medium, at any time.

The average values calculated above have clearly a

straightforward interpretation. In order to avoid the necessity of putting in place of $\xi_k{}^{(1)}$ the coordinate x_k of the point of observation, $\xi_k{}^{(1)}$ will be identified with x_k and will be written ξ_k. Then

$$g(\xi_k,t) = \bar{G}(\xi_k,t) = \frac{2m}{\omega}\int [f_1]d_{(3)}\rho^{(1)}, \qquad (2.9)$$

$$g(\xi_k,t)u_l(\xi_k,t) = \bar{I}_l(\xi_k,t) = -\frac{i\hbar}{\omega}\int \left[\frac{\partial f_1}{\partial \eta_l{}^{(1)}}\right]d_{(3)}\rho^{(1)}, \quad (2.10)$$

$$g(\xi_k,t)m_l(\xi_k,t) = \bar{M}_l(\xi_k,t) - \epsilon_{lmn}g\xi_m u_n$$

$$= -\frac{i\hbar}{\omega}\int \epsilon_{lmn}\rho_m{}^{(1)}\left[\frac{\partial f_1}{\partial \sigma_n{}^{(1)}}\right]d_{(3)}\rho, \quad (2.11)$$

$$\tfrac{1}{2}g(\xi_k,t)u_l(\xi_k,t)u_l(\xi_k,t)$$

$$+\tfrac{1}{2}g(\xi_k,t)m_l(\xi_k,t)\omega_l(\xi_k,t) + g(\xi_k,t)\epsilon(\xi_k,t)$$

$$= \bar{E}(\xi_k,t) = -\frac{\hbar^2}{m\omega}\int\left[\frac{\partial^2 f_1}{\partial \sigma_l{}^{(1)}\partial \sigma_l{}^{(1)}} + \frac{1}{4}\frac{\partial^2 f_1}{\partial \eta_l{}^{(1)}\partial \eta_l{}^{(1)}}\right.$$

$$\left.+\frac{1}{16}\frac{\partial^2 f_1}{\partial \xi_l\partial \xi_l}\right]d_{(3)}\rho^{(1)} + \frac{1}{\omega}\int [\phi_{1'1'}f_1]d_{(3)}\rho^{(1)}$$

$$+\frac{1}{2\omega^2}\int [\phi_{1'2'}f_2]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}. \quad (2.12)$$

3. METHOD OF SOLUTION OF THE EQUATIONS OF MOTION FOR THE DISTRIBUTION OPERATORS BY MEANS OF A SERIES EXPANSION

To calculate the hydrodynamic variables the f_1 and f_2 functions are needed. Therefore some method of solution of Eq. (1.4) must be given. We are interested in the so-called normal solutions, i.e., in solutions which are uniquely determined by specifying hydrodynamic variables throughout the domain of the fluid (see Green[10]).

Instead of specifying the values of hydrodynamic variables throughout the domain of the fluid, the values of hydrodynamic variables and their spatial derivatives at given point may be applied. In this case the Taylor's expansion of hydrodynamic variables in the vicinity of a given point is used. Then the functions f_s must comply with the following conditions:

(1) They do not depend explicitly on ξ_k, because the spatial dependence of the f_s functions is included in the

[10] H. S. Green, *Molecular Theory of Fluids* (Interscience Publishers, Inc., New York, 1952).

dependence of the hydrodynamic variables on the ξ_k. This situation does not vary on passing to the specification of these variables and their spatial derivatives at a given point.

(2) They do not depend explicitly on the time, because in the normal state the dependence on the time is caused entirely by the time dependence of the hydrodynamic variables and their spatial derivatives which are arguments of f_s functions.

Further on it has been assumed that we are interested only in such states in which the gradients of hydrodynamic variables and the higher derivatives of these quantities are quite small. Then it is possible to expand the f_s functions in the Taylor series

$$f_s = f_s{}^{(0)} + f_s{}^{(1)} + f_s{}^{(2)} + \cdots, \qquad (3.1)$$

where the $f_s{}^{(0)}$ do not depend on the derivatives of hydrodynamic variables, the $f_s{}^{(1)}$ are linear in their first derivatives, the $f_s{}^{(2)}$ are quadratic in the first derivatives and linear in second derivatives, and so on. It may be said that the first term of this expansion describes the state of the fluid which is determined only by the values of hydrodynamic variables but not by their derivatives. To see whether this is a solution corresponding to thermodynamic equilibrium, one must find the integro-differential equation which this term must satisfy.

Taking into account the postulate formulated above, the derivatives which are in Eq. (1.4) may be written in the form:

$$\frac{\partial f_s}{\partial t} = \frac{\partial f_s}{\partial a_k}\frac{\partial a_k}{\partial t} + \frac{\partial f_s}{\partial a_k/\partial \xi_l}\frac{\partial^2 a_k}{\partial t\partial \xi_l} + \cdots \qquad (3.2)$$

$$\frac{\partial^2 f_s}{\partial \xi_i\partial \eta_i{}^{(1)}} = \frac{\partial}{\partial \eta_i{}^{(1)}}\frac{\partial f_s}{\partial a_k}\frac{\partial a_k}{\partial \xi_i}$$

$$+\frac{\partial}{\partial \eta_i{}^{(1)}}\frac{\partial f_s}{\partial a_k/\partial \xi_l}\frac{\partial^2 a_k}{\partial \xi_i\partial \xi_l} + \cdots. \qquad (3.3)$$

To expand Eq. (1.4) into a system of equations, one must know the manner in which the expression $\partial a_k/\partial t$ expand with respect to the derivatives $\partial a_k/\partial \xi_l$, where now the a_k stand for all the hydrodynamic variables of interest. For this purpose the general form of the hydrodynamic equations must be calculated.

4. GENERAL FORM OF HYDRODYNAMICAL EQUATIONS

Let us calculate the time derivatives from Eqs. (2.9) to (2.12), which are needed in the calculation of the

hydrodynamic equations:

$$\frac{\partial g(\xi_k,t)}{\partial t}=\frac{\partial}{\partial t}\left\{\frac{2m}{\omega}\int[f_1]d_{(3)}\rho^{(1)}\right\}=\frac{2m}{\omega}\int\left[\frac{\partial f_1}{\partial t}\right]d_{(3)}\rho^{(1)}, \tag{4.1}$$

$$\frac{\partial g(\xi_k,t)u_l(\xi_k,t)}{\partial t}=\frac{\partial}{\partial t}\left\{-\frac{i\hbar}{\omega}\int\left[\frac{\partial f_1}{\partial\eta_l^{(1)}}\right]d_{(3)}\rho^{(1)}\right\}=-\frac{i\hbar}{\omega}\int\left[\frac{\partial}{\partial\eta_l^{(1)}}\frac{\partial f_1}{\partial t}\right]d_{(3)}\rho^{(1)}, \tag{4.2}$$

$$\frac{\partial g(\xi_k,t)m_l(\xi_k,t)}{\partial t}=\frac{\partial}{\partial t}\left\{-\frac{i\hbar}{\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial f_1}{\partial\sigma_n^{(1)}}\right]d_{(3)}\rho^{(1)}\right\}=-\frac{i\hbar}{\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial}{\partial\sigma_n^{(1)}}\frac{\partial f_1}{\partial t}\right]d_{(3)}\rho^{(1)} \tag{4.3}$$

$$\frac{\partial}{\partial t}\{\tfrac{1}{2}gu^2+\tfrac{1}{2}gm_l\omega_l+g\epsilon\}=-\frac{\hbar^2}{m\omega}\int\left[\frac{\partial^2}{\partial\sigma_k^{(1)}\partial\sigma_k^{(1)}}\frac{\partial f_1}{\partial t}+\frac{1}{4}\frac{\partial^2}{\partial\eta_k^{(1)}\partial\eta_k^{(1)}}\frac{\partial f_1}{\partial t}\right.$$

$$\left.+\frac{1}{16}\frac{\partial^2}{\partial\xi_k\partial\xi_k}\frac{\partial f_1}{\partial t}\right]d_{(3)}\rho^{(1)}+\frac{1}{\omega}\int\left[\phi_{1'1'}\frac{\partial f_1}{\partial t}\right]d_{(3)}\rho^{(1)}+\frac{1}{2\omega^2}\int\left[\phi_{1'2'}\frac{\partial f_2}{\partial t}\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}. \tag{4.4}$$

If now the equations of motion for the f_s functions are used, the successive hydrodynamic equations may be obtained. First, the equation of continuity is given by

$$\frac{\partial g(\xi_k,t)}{\partial t}=\frac{2m}{\omega}\int\left[\frac{2i\hbar}{m}\frac{\partial^2 f_1}{\partial\rho_i^{(1)}\partial\sigma_i^{(1)}}+\frac{i\hbar}{2m}\frac{\partial^2 f_1}{\partial\xi_i\partial\eta_i^{(1)}}+\frac{1}{i\hbar}(\phi_{1'1'}-\phi_{1''1''})f_1+\frac{1}{\omega i\hbar}\int\{(\phi_{1'2''}-\phi_{1''2''})f_2\}_{\eta_k^{(2)}=\sigma_k^{(2)}=0}\right.$$

$$\left.\times d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}\right]d_{(3)}\rho^{(1)}=\frac{i\hbar}{\omega}\frac{\partial}{\partial\xi_i}\int\left[\frac{\partial f_1}{\partial\eta_i^{(1)}}\right]d_{(3)}\rho^{(1)}=-\frac{\partial}{\partial\xi_i}g(\xi_k,t)u_i(\xi_k,t). \tag{4.5}$$

When deriving the momentum equation one must take into account the following property of the f_s functions. As the system of molecules obeys Bose statistics, it may be written

$$P_{ij}F_s=F_sP_{ij}=F_s, \tag{4.6}$$

where P_{ij} is a permutation operator of molecules "i" and "j". This property is transferred without change to the f_s functions. It may be written, e.g., for $s=2$:

$$f_2(\xi_k,\rho_k^{(1)},\eta_k^{(1)},\sigma_k^{(1)},\xi_k^{(2)},\rho_k^{(2)},\eta_k^{(2)},\sigma_k^{(2)})$$
$$=f_2(\xi_k+\xi_k^{(2)},\rho_k^{(2)},\eta_k^{(2)},\sigma_k^{(2)},$$
$$-\xi_k^{(2)},\rho_k^{(1)},\eta_k^{(1)},\sigma_k^{(1)}). \tag{4.7}$$

Moreover, the following relation may be written:

$$f_s(\xi_k,\rho_k^{(1)},\eta_k^{(1)},\sigma_k^{(1)},\cdots,\xi_k^{(i)},\rho_k^{(i)},\eta_k^{(i)},\sigma_k^{(i)},\cdots)$$
$$=f_s(\xi_k,\rho_k^{(1)},\eta_k^{(1)},\sigma_k^{(1)},\cdots,\xi_k^{(i)},$$
$$-\rho_k^{(i)},\eta_k^{(i)},-\sigma_k^{(i)},\cdots), \tag{4.8}$$

which stems from the identity of atoms of our diatomic molecule; and the form of the potentials ϕ_{11} and ϕ_{12} may be specified:

$$\phi_{11}=\phi_{11}(|r^{(1)}|), \tag{4.9}$$

$$\phi_{12}=v(|R^{(1)}-R^{(2)}+\tfrac{1}{2}(r^{(1)}-r^{(2)})|)$$
$$+v(|R^{(1)}-R^{(2)}+\tfrac{1}{2}(r^{(1)}+r^{(2)})|)$$
$$+v(|R^{(1)}-R^{(2)}-\tfrac{1}{2}(r^{(1)}+r^{(2)})|)$$
$$+v(|R^{(1)}-R^{(2)}-\tfrac{1}{2}(r^{(1)}-r^{(2)})|), \tag{4.10}$$
$$|r^{(1)}|\equiv(r_k^{(1)}r_k^{(1)})^{\frac{1}{2}}.$$

Then the following relations are of interest, and are easily available from formulas (4.9) and (4.10):

$$\left[\frac{\partial}{\partial\sigma_l^{(1)}}(\phi_{1'1'}-\phi_{1''1''})\right]=\frac{\partial}{\partial\rho_l^{(1)}}[\phi_{1'1'}]\equiv\frac{\partial\phi(1.1)}{\partial\rho_l^{(1)}}=\frac{\partial\phi(1.1)}{\partial|\rho^{(1)}|}\frac{\rho_l^{(1)}}{|\rho^{(1)}|},$$

$$\left[\frac{\partial\phi_{1'2''}}{\partial\eta_k^{(1)}}-\frac{\partial\phi_{1''2''}}{\partial\eta_k^{(1)}}\right]=-\frac{\partial}{\partial\xi_k^{(2)}}[\phi_{1'2''}]=-\frac{\partial}{\partial\xi_k^{(2)}}[\phi_{1''2''}]\equiv-\frac{\partial\phi(1.2)}{\partial\xi_k^{(2)}}, \tag{4.11}$$

$$\left[\frac{\partial\phi_{1'2''}}{\partial\sigma_k^{(1)}}-\frac{\partial\phi_{1''2''}}{\partial\sigma_k^{(1)}}\right]=\frac{\partial}{\partial\rho_k^{(1)}}[\phi_{1'2''}]=\frac{\partial}{\partial\rho_k^{(1)}}[\phi_{1''2''}]\equiv\frac{\partial\phi(1.2)}{\partial\rho_k^{(1)}}.$$

From these facts we obtain: the equation of momentum,

$$g(\xi_k,t)\frac{\partial u_l(\xi_k,t)}{\partial t} = -g(\xi_k,t)u_j(\xi_k,t)\frac{\partial u_l(\xi_k,t)}{\partial \xi_j} + \frac{\partial}{\partial \xi_j}T_{lj}, \tag{4.12}$$

where

$$T_{lj} = g(\xi_k,t)u_l(\xi_k,t)u_j(\xi_k,t) + \frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 f_1}{\partial \eta_l^{(1)}\partial \eta_j^{(1)}}\right]d_{(3)}\rho^{(1)} + \frac{1}{2\omega^2}\int\frac{\partial \phi(1.2)}{\partial \xi_l^{(2)}}\xi_j^{(2)}$$

$$\times\left[f_2 - \frac{1}{2!}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \frac{1}{3!}\xi_i^{(2)}\xi_n^{(2)}\frac{\partial^2 f_2}{\partial \xi_i\partial \xi_n} - \cdots\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}; \tag{4.13}$$

the equation of angular momentum,

$$g\frac{\partial m_l(\xi_k,t)}{\partial t} = -gu_j\frac{\partial m_l(\xi_k,t)}{\partial \xi_j} + \frac{\partial}{\partial \xi_j}Q_{lj} - \epsilon_{lmn}T_{mn}, \tag{4.14}$$

with

$$Q_{lj} = g(\xi_k,t)u_j(\xi_k,t)m_l(\xi_k,t) + \frac{\hbar^2}{2m\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial^2 f_1}{\partial \eta_j^{(1)}\partial \sigma_n^{(1)}}\right]d_{(3)}\rho^{(1)} + \frac{1}{\omega^2}\int\epsilon_{lmn}v'\frac{\rho_m^{(2)}\xi_n^{(2)}\xi_j^{(2)}+\frac{1}{2}\rho_n^{(1)}\rho_m^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}$$

$$\times\left[f_2 - \frac{1}{2!}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \cdots\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{1}{\omega^2}\int\epsilon_{lmn}v'\frac{(\rho_m^{(1)}+\rho_m^{(2)})\xi_n^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}$$

$$\times\left[\frac{1}{2!}f_2 - \frac{1}{3!}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \cdots\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}$$

$$v' \equiv \frac{d}{d|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}v(|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|); \tag{4.15}$$

and the equation of energy,

$$\frac{\partial}{\partial t}\{\tfrac{1}{2}gu^2 + ge_r + g\epsilon\} = -\frac{\partial}{\partial \xi_j}\left\{gu_j\left(\frac{u^2}{2}+e_r+\epsilon\right)\right\} + (u_kT_{kj}),_j + (\omega_kQ_{kj}+q_j),_j \tag{4.16}$$

$$e_r \equiv \tfrac{1}{2}m_l\omega_l,$$

where

$$q_j = u_j(g\epsilon - \tfrac{1}{2}gu^2 - ge_r) - \frac{i\hbar^3}{2m^2\omega}\int\left[\frac{\partial}{\partial \eta_j^{(1)}}\left(\frac{\partial^2 f_1}{\partial \sigma_i^{(1)}\partial \sigma_i^{(1)}} + \frac{1}{4}\frac{\partial^2}{\partial \eta_i^{(1)}\partial \eta_i^{(1)}} + \frac{1}{16}\frac{\partial^2 f_1}{\partial \xi_i\partial \xi_i}\right)\right]d_{(3)}\rho^{(1)}$$

$$+ \frac{i\hbar}{2m\omega}\int\left[\phi(1.1)\frac{\partial f_1}{\partial \eta_j^{(1)}}\right]d_{(3)}\rho^{(1)} + \frac{i\hbar}{4m\omega^2}\left[\int\phi(1.2)\frac{\partial f_2}{\partial \eta_j^{(1)}}\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{i\hbar}{8m\omega^2}\int\frac{\partial\phi(1.2)}{\partial \xi_i^{(2)}}\xi_j^{(2)}$$

$$\times\left[\left(\frac{\partial}{\partial \eta_i^{(1)}} + \frac{\partial}{\partial \eta_i^{(2)}}\right)\left(f_2 - \tfrac{1}{2}\xi_n^{(2)}\frac{\partial f_2}{\partial \xi_n} + \cdots\right)\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{2}{\omega^2}\int v'\frac{\xi_k^{(2)}+\frac{1}{2}(\rho_k^{(1)}+\rho_k^{(2)})}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\xi_j^{(2)}u_k$$

$$\times\left[f_2 - \tfrac{1}{2}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \cdots\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 f_1}{\partial \eta_k^{(1)}\partial \eta_j^{(1)}}\right]u_kd_{(3)}\rho^{(1)} - \frac{\hbar^2}{2m\omega}\int\epsilon_{kmn}\rho_m^{(1)}$$

$$\times\left[\frac{\partial^2 f_1}{\partial \eta_j^{(1)}\partial \sigma_n^{(1)}}\right]\omega_kd_{(3)}\rho^{(1)} - \frac{1}{\omega^2}\int\epsilon_{kmn}v'\omega_k\frac{\rho_m^{(2)}\xi_n^{(2)}\xi_j^{(2)}+\frac{1}{2}\rho_n^{(1)}\rho_m^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\left[f_2 - \frac{1}{2!}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \cdots\right]$$

$$\times d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} + \frac{1}{\omega^2}\int\epsilon_{kmn}v'\omega_k\frac{(\rho_m^{(1)}+\rho_m^{(2)})\xi_n^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\left[\frac{1}{2!}f_2 - \frac{1}{3!}\xi_i^{(2)}\frac{\partial f_2}{\partial \xi_i} + \cdots\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}. \tag{4.17}$$

Using the expansion of the f_s functions given in the preceding paragraph, one may expand also the quantities T_{lj}, Q_{lj}, and q_j as a series of derivatives of hydrodynamic variables:

$$T_{lj} = T_{lj}^{(0)} + T_{lj}^{(1)} + T_{lj}^{(2)} + \cdots, \quad Q_{lj} = Q_{lj}^{(0)} + Q_{lj}^{(1)} + Q_{lj}^{(2)} + \cdots, \quad q_j = q_j^{(0)} + q_j^{(1)} + q_j^{(2)} + \cdots, \tag{4.18}$$

where

$$T_{lj}^{(0)} = gu_lu_j + \frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 f_1^{(0)}}{\partial\eta_l^{(1)}\partial\eta_j^{(1)}}\right]d_{(3)}\rho^{(1)} + \frac{2}{\omega^2}\int v'\frac{\frac{1}{2}(\rho_l^{(1)}+\rho_l^{(2)})\xi_j^{(2)}+\xi_l^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}[f_2^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (4.19)$$

$$T_{lj}^{(1)} = \frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 f_1^{(1)}}{\partial\eta_l^{(1)}\partial\eta_j^{(1)}}\right]d_{(3)}\rho^{(1)} + \frac{1}{\omega^2}\int v'\frac{\frac{1}{2}(\rho_l^{(1)}+\rho_l^{(2)})\xi_j^{(2)}+\xi_l^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}$$

$$\times\left[f_2^{(1)}-\frac{1}{2}\xi_n^{(2)}\frac{\partial f_2^{(0)}}{\partial\xi_n}\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (4.20)$$

$$Q_{lj}^{(0)} = gu_jm_l + \frac{\hbar^2}{2m\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial^2 f_1^{(0)}}{\partial\eta_j^{(1)}\partial\sigma_n^{(1)}}\right]d_{(3)}\rho^{(1)}$$

$$-\frac{1}{2\omega^2}\int\epsilon_{lmn}v'\frac{(\rho_m^{(1)}-\rho_m^{(2)})\xi_n^{(2)}+\rho_m^{(1)}\rho_n^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\xi_j^{(2)}[f_2^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (4.21)$$

$$Q_{lj}^{(1)} = \frac{\hbar^2}{2m\omega}\int\epsilon_{lmn}\rho_m^{(1)}\left[\frac{\partial^2 f_1^{(1)}}{\partial\eta_j^{(1)}\partial\sigma_n^{(1)}}\right]d_{(3)}\rho^{(1)} - \frac{1}{2\omega^2}\int\epsilon_{lmn}v'\frac{(\rho_m^{(1)}-\rho_m^{(2)})\xi_n^{(2)}+\rho_m^{(1)}\rho_n^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}$$

$$\times\xi_j^{(2)}[f_2^{(1)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{1}{2\omega^2}\int\epsilon_{lmn}v'\frac{\rho_m^{(2)}\xi_n^{(2)}\xi_j^{(2)}+\frac{1}{2}\rho_n^{(1)}\rho_m^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}$$

$$\times\left[\xi_n^{(2)}\frac{\partial f_2^{(0)}}{\partial\xi_n}\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} + \frac{1}{6\omega^2}\int\epsilon_{lmn}v'\frac{(\rho_m^{(1)}+\rho_m^{(2)})\xi_n^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\left[\xi_n^{(2)}\frac{\partial f_2^{(0)}}{\partial\xi_n}\right]$$

$$\times d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (4.22)$$

$$q_j^{(0)} = u_j(g\epsilon - ge_r - \frac{1}{2}gu^2) - \frac{i\hbar}{2m^2\omega}\int\int\left[\frac{\partial}{\partial\eta_j^{(1)}}\left(\frac{\partial^2 f_1^{(0)}}{\partial\sigma_i^{(1)}\partial\sigma_i^{(1)}}+\frac{1}{4}\frac{\partial^2 f_1^{(0)}}{\partial\eta_i^{(1)}\partial\eta_i^{(1)}}\right)\right]d_{(3)}\rho^{(1)} + \frac{i\hbar}{2m\omega}\int\left[\phi(1.1)\frac{\partial f_1^{(0)}}{\partial\eta_j^{(1)}}\right]d_{(3)}\rho^{(1)}$$

$$+\frac{i\hbar}{4m\omega}\int\left[\phi(1.2)\frac{\partial f_2^{(0)}}{\partial\eta_j^{(1)}}\right]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{i\hbar}{8m\omega^2}\int\frac{\partial\phi(1.2)}{\partial\xi_i^{(2)}}\xi_j^{(2)}\left[\left(\frac{\partial}{\partial\eta_i^{(1)}}+\frac{\partial}{\partial\eta_i^{(2)}}\right)f_2^{(0)}\right]$$

$$\times d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)} - \frac{2}{\omega^2}\int\xi_j^{(2)}u_kv'\frac{\xi_k^{(2)}+\frac{1}{2}(\rho_k^{(1)}+\rho_k^{(2)})}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}[f_2^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}$$

$$-\frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 f_1^{(0)}}{\partial\eta_k^{(1)}\partial\eta_j^{(1)}}\right]u_kd_{(3)}\rho^{(1)} - \frac{\hbar^2}{2m\omega}\int\epsilon_{kmn}\rho_m^{(1)}\left[\frac{\partial^2 f_1^{(0)}}{\partial\eta_j^{(1)}\partial\sigma_n^{(1)}}\right]\omega_kd_{(3)}\rho^{(1)}$$

$$-\frac{1}{\omega^2}\int\epsilon_{kmn}v'\omega_k\frac{\rho_m^{(2)}\xi_n^{(2)}\xi_j^{(2)}+\frac{1}{2}\rho_n^{(1)}\rho_m^{(2)}\xi_j}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}[f_2^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}$$

$$+\frac{1}{2\omega^2}\int\epsilon_{kmn}v'\omega_k\frac{(\rho_m^{(1)}+\rho_m^{(2)})\xi_n^{(2)}\xi_j^{(2)}}{|\xi^{(2)}+\frac{1}{2}(\rho^{(1)}+\rho^{(2)})|}[f_2^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}, \quad (4.23)$$

and so on.

5. INTEGRO-DIFFERENTIAL EQUATIONS FOR THE EXPANSION COEFFICIENTS OF f_s FUNCTIONS

As is easily seen from the general form of the hydrodynamic equations and the formulas for T_{lj}, Q_{lj}, q_j derived above, all the quantities $\partial a_k/\partial t$ which are in Eqs. (3.2) begin with the term linear with respect to the gradients of a_k, with the exception of

$$g\partial m_k/\partial t = -gu_im_{\kappa,i} + Q_{kj,j}^{(0)} - \epsilon_{kmn}T_{mn}^{(0)} + \cdots, \quad (5.1)$$

where the term $\epsilon_{kmn}T_{mn}^{(0)}$ is of zero order. This term vanishes in the case of central intermolecular forces. For this reason the integro-differential equations determining the zeroth term of the expansion of the f_s functions in series have the form

$$\frac{2i\hbar}{m}\left\{\sum_{i=1}^{s}\frac{\partial^2 f_s{}^{(0)}}{\partial\rho_k{}^{(i)}\sigma_k{}^{(i)}}-\tfrac{1}{4}\sum_{i=2}^{s}\left(\frac{\partial^2 f_s{}^{(0)}}{\partial\eta_k{}^{(1)}\partial\xi_k{}^{(i)}}-\frac{\partial^2 f_s{}^{(0)}}{\partial\eta_k{}^{(i)}\partial\xi_k{}^{(i)}}\right)\right\}+\frac{1}{i\hbar}\sum_{i\leqslant j}^{s}(\phi_{i'j'}-\phi_{i''j''})f_s{}^{(0)}$$

$$+\frac{1}{\omega i\hbar}\sum_{i=1}^{s}\int\left[(\phi_{i',\,(s+1)''}-\phi_{i'',\,(s+1)''})f_{s+1}{}^{(0)}\right]_{\eta_k{}^{(s+1)}=\sigma_k{}^{(s+1)}=0}d_{(3)}\rho^{(s+1)}d_{(3)}\xi^{(s+1)}=-\frac{1}{g}\epsilon_{kmn}T_{mn}{}^{(0)}\frac{\partial f_s{}^{(0)}}{\partial m_k}$$

$$\equiv-\frac{1}{g\omega^2}\frac{\partial f_s{}^{(0)}}{\partial m_k}\int\epsilon_{kmn}v'\frac{(\rho_m{}^{(1)}+\rho_m{}^{(2)})\xi_n{}^{(0)}}{|\xi^{(2)}+\tfrac{1}{2}(\rho^{(1)}+\rho^{(2)})|}[f_2{}^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}.\quad(5.2)$$

From this equation it may be seen that $f_s{}^{(0)}$ does not correspond to the thermodynamic equilibrium. $f_s{}^{(0)}$ is the equilibrium solution only in a case when the right side of the equation vanishes. This takes place, for example, in the case of a central intermolecular potential. Not excluded is also the possibility that for the equilibrium solution the right side of this equation vanishes, but to date no proof of this fact has been found.

Now the integro-differential equations determining the first term of the expansion of the f_s functions have the following form:

$$\frac{2i\hbar}{m}\left\{\sum_{i=1}^{s}\frac{\partial^2 f_s{}^{(1)}}{\partial\rho_k{}^{(i)}\partial\sigma_k{}^{(i)}}-\tfrac{1}{4}\sum_{i=2}^{s}\left(\frac{\partial^2 f_s{}^{(1)}}{\partial\eta_k{}^{(1)}\partial\xi_k{}^{(i)}}-\frac{\partial^2 f_s{}^{(1)}}{\partial\eta_k{}^{(i)}\partial\xi_k{}^{(i)}}\right)\right\}+\frac{1}{i\hbar}\sum_{i\leqslant j}^{s}(\phi_{1'1'}-\phi_{1''1''})f_s{}^{(1)}$$

$$+\frac{1}{\omega i\hbar}\sum_{i=1}^{s}\int\left[(\phi_{i',\,(s+1)''}-\phi_{i'',\,(s+1)''})f_{s+1}{}^{(1)}\right]_{\eta_k{}^{(s+1)}=\sigma_k{}^{(s+1)}=0}d_{(3)}\rho^{(s+1)}d_{(3)}\xi^{(s+1)}=-\frac{i\hbar}{2m}\frac{\partial}{\partial\eta_k{}^{(1)}}\frac{\partial f_s{}^{(0)}}{\partial a_i}\frac{\partial a_i}{\partial\xi_k}$$

$$+\frac{\partial f_s{}^{(0)}}{\partial a_i}\frac{\partial a_i}{\partial t}+\frac{1}{g}\epsilon_{imn}T_{mn}{}^{(1)}\frac{\partial f_s{}^{(1)}}{\partial m_i}+\frac{\partial f_s{}^{(1)}}{\partial m_k/\partial\xi_i}\frac{\partial}{\partial\xi_i}\left(-\frac{1}{g}\epsilon_{kmn}T_{mn}{}^{(0)}\right).\quad(5.3)$$

In a similar manner the integro-differential equations for the higher expansion coefficients of the f_s functions may be easily written.

The equations described above do not determine uniquely the expansion coefficients of the f_s functions. The following requirements must be added:

(1) The zeroth expansion coefficients must give all the hydrodynamic variables,

$$g(\xi_k,t)=\frac{2m}{\omega}\int[f_1{}^{(0)}]d_{(3)}\rho^{(1)},\quad\int[f_1{}^{(k)}]d_{(3)}\rho^{(1)}=0,\quad(5.4)$$

$$g(\xi_k,t)u_l(\xi_k,t)=-\frac{i\hbar}{\omega}\int\left[\frac{\partial f_1{}^{(0)}}{\partial\eta_l{}^{(1)}}\right]d_{(3)}\rho^{(1)},\quad\int\left[\frac{\partial f_1{}^{(k)}}{\partial\eta_l{}^{(1)}}\right]d_{(3)}\rho^{(1)}=0,\quad(5.5)$$

$$g(\xi_k,t)m_l(\xi_k,t)=-\frac{i\hbar}{\omega}\int\epsilon_{lmn}\rho_m{}^{(1)}\left[\frac{\partial f_1{}^{(0)}}{\partial\sigma_n{}^{(1)}}\right]d_{(3)}\rho^{(1)},\quad\int\epsilon_{lmn}\rho_m{}^{(1)}\left[\frac{\partial f_1{}^{(k)}}{\partial\sigma_n{}^{(1)}}\right]d_{(3)}\rho^{(1)}=0,\quad(5.6)$$

$$\tfrac{1}{2}gu^2+ge_r+g\epsilon=-\frac{\hbar^2}{m\omega}\int\left[\frac{\partial^2 f_1{}^{(0)}}{\partial\sigma_k{}^{(1)}\partial\sigma_k{}^{(1)}}+\frac{1}{4}\frac{\partial^2 f_1{}^{(0)}}{\partial\eta_k{}^{(1)}\partial\eta_k{}^{(1)}}\right]d_{(3)}\rho^{(1)}+\frac{1}{\omega}\int[\phi(1.1)f_1{}^{(0)}]d_{(3)}\rho^{(1)}$$

$$+\frac{1}{2\omega^2}\int[\phi(1.2)f_2{}^{(0)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)};$$

$$-\frac{\hbar^2}{m\omega}\int\left[\frac{\partial^2 f_1{}^{(k)}}{\partial\sigma_i{}^{(1)}\partial\sigma_i{}^{(1)}}+\frac{1}{4}\frac{\partial^2 f_1{}^{(k)}}{\partial\eta_i{}^{(1)}\partial\eta_i{}^{(1)}}+\frac{1}{16}\frac{\partial^2 f^{(k-2)}}{\partial\xi_i\partial\xi_i}\right]d_{(3)}\rho^{(1)}+\frac{1}{\omega}\int[\phi(1.1)f_1{}^{(k)}]d_{(3)}\rho^{(1)}$$

$$+\frac{1}{2\omega^2}\int[\phi(1.2)f_2{}^{(k)}]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}=0,\quad(k=1,2,\cdots).\quad(5.7)$$

(2) The condition of the decrease of correlation must be also split with respect to the gradients of hydrodynamic variables,

$$f_2^{(0)} \xrightarrow[(\xi_k^{(2)}\xi_k^{(2)})^{\frac{1}{2}} \to \infty]{} f_1^{(0)} f_1^{(0)},$$

$$f_2^{(1)} \xrightarrow[(\xi_k^{(2)}\xi_k^{(2)})^{\frac{1}{2}} \to \infty]{} f_1^{(0)} f_1^{(1)} + f_1^{(1)} f_1^{(0)}, \cdots. \quad (5.8)$$

6. HYDRODYNAMIC EQUATIONS OF THE ZEROTH APPROXIMATION

The equation of the zeroth approximation from the preceding paragraph may be treated in a manner similar to the classical case, i.e., the right side of the equation may be treated as a small perturbation (which vanishes, as we know, in the case of a central intermolecular potential). For these purposes we may attach to it the parameter λ and expand the $f_s^{(0)}$ with respect to this parameter:

$$f_s^{(0)} = f_s^{(00)} + f_s^{(01)} + f_s^{(02)} + \cdots. \quad (6.1)$$

Now it must be required that $f_s^{(00)}$ gives also all the hydrodynamic variables. It is the solution of the equation of equilibrium. Some information with respect to its form may be obtained from considerations of Gibbs distributions, as was done for the classical case.[8] But the known methods of calculation of the Gibbs distribution, based on the development with respect to the powers of $\hbar$, are not suitable for our problem and give enormously complicated results. For this reason we must now give up the attempt at effective calculation of the $f_s^{(0)}$ functions or the $f_s^{(00)}$ functions and limit ourselves only to the qualitative analysis of the solutions of the equations in the zeroth approximation. With this in mind, let us introduce the functions r_s. These are the solutions of the equations of equilibrium in the case $u_k = \omega_k = 0$ (the case of the rest of our system) for given density and intrinsic energy g, ϵ. Since for gases at normal temperatures the equations of equilibrium have only one solution, the r_s functions must be invariant with respect to all transformations for which the equations of equilibrium remain invariant.

Such transformations are: (a) the rotation and translation of the coordinate system, (b) the transformation $\eta_k^{(i)} \to -\eta_k^{(i)}$, $\sigma_k^{(i)} \to -\sigma_k^{(i)}$, and (c) the space reflections ($\rho_k^{(i)}$, $\sigma_k^{(i)}$, $\eta_k^{(i)}$, $\xi_k^{(i)}$ change the signs of all components or some of these components).

The r_s with such properties do give definite values of g and ϵ and $u_k = \omega_k = 0$. The stress tensor for the r_1 and r_2 functions reduces to the diagonal form and defines the pressure. Hence the r_s functions are special solutions of the zeroth approximation equations (5.2) (because the antisymmetric part of the stress tensor vanishes). Therefore the solutions of Eqs. (5.2) fulfilling the conditions (5.4) to (5.7) are assumed to have the form

$$f_s^{(0)} = \exp[(i/\hbar)h_s^{(0)}]r_s. \quad (6.2)$$

The knowledge of the $h_s^{(0)}$ may be limited to only a few terms of the following Taylor expansion:

$$h_s^{(0)} = [h_s^{(0)}] + \sum_{k=1}^{s} (\alpha_i^{(k)}\eta_i^{(k)} + \beta_i^{(k)}\sigma_i^{(k)} + \gamma_{ij}^{(k)}\sigma_i^{(k)}\eta_j^{(k)} + \alpha_{ij}^{(k)}\eta_i^{(k)}\eta_j^{(k)} + \beta_{ij}^{(k)}\sigma_i^{(k)}\sigma_j^{(k)} + \cdots). \quad (6.3)$$

It may be easily seen that the first term of the development is responsible for the changes of density and energy, which are caused by the existence of the velocities u_k and ω_k. Using the conditions (5.5) and (5.6), the following relations for the $h_1^{(0)}$ expansion coefficients are obtained:

$$g(\xi_k,t)u_l(\xi_k,t)$$
$$= \frac{1}{\omega}\int \alpha_l^{(1)}[r_1] \exp[(i/\hbar)h_1^{(0)}]d_{(3)}\rho^{(1)}, \quad (6.4)$$

from which, using

$$\frac{2m}{\omega}\int [r_1] \exp[(i/\hbar)h_1^{(0)}]d_{(3)}\rho^{(1)} = g$$

we obtain

$$\alpha_l^{(1)} = 2mu_l, \quad (6.5)$$

and

$$g(\xi_k,t)m_l(\xi_k,t)$$
$$= \frac{1}{\omega}\int \epsilon_{lmn}\rho_m^{(1)}\beta_n^{(1)}[r_1] \exp[(i/\hbar)h_1^{(0)}]d_{(3)}\rho^{(1)}. \quad (6.6)$$

In order to use the last condition, we introduce into our considerations a new operator: the operator of the moment of inertia of the fluid at given point x:

$$I_{kl}(x_s) = \sum_{i=1}^{N} m\{\epsilon_{kpq}\tfrac{1}{2}r_p^{(i)}\epsilon_{ltq}\tfrac{1}{2}r_t^{(i)}\delta_{(3)}(R_s^{(i)} - x_s) + \delta_{(3)}(R_s^{(i)} - x_s)\epsilon_{kpq}\tfrac{1}{2}r_p^{(i)}\epsilon_{ltq}\tfrac{1}{2}r_t^{(i)}\}. \quad (6.7)$$

The average value of this operator has the form

$$\bar{I}_{kl}(x_s,t) = \frac{m}{2\omega}\int \epsilon_{kpq}\rho_p^{(1)}\epsilon_{ltq}\rho_t^{(1)}[f_1]d_{(3)}\rho^{(1)}, \quad (6.8)$$

by means of which the density of inertia tensor of the fluid at the point ξ_k and the time t is defined:

$$i_{kl}(\xi_k,t) = \frac{m}{2\omega}\int \epsilon_{kpq}\rho_p^{(1)}\epsilon_{ltq}\rho_t^{(1)}[f_1]d_{(3)}\rho^{(1)}. \quad (6.9)$$

The above-mentioned condition may be written in the form

$$i_{kl}(\xi_k,t)\omega_l(\xi_k,t)$$
$$= \frac{1}{\omega}\int \epsilon_{kmn}\rho_m^{(1)}\beta_n^{(1)}[r_1] \exp[(i/\hbar)h_1^{(0)}]d_{(3)}\rho^{(1)}, \quad (6.10)$$

from which it follows that

$$\beta_n^{(1)} = (m/2)\epsilon_{ltn}\rho_t^{(1)}\omega_l(\xi_k,t). \quad (6.11)$$

In this manner we have two terms of the Taylor expansion of the $h_1^{(0)}$ function; the remaining coefficients are the unknown functions of u_k and ω_k, which for $u_k=\omega_k=0$ ought to vanish identically. Writing equations for the functions $h_s^{(0)}$ from the Eqs. (5.2) is naturally a trivial operation. Using the expansion of the $h_s^{(0)}$ functions, we may calculate the forms of $T_{kl}^{(0)}$, $Q_{kl}^{(0)}$ and $q_k^{(0)}$ according to formulas (4.19) and (4.21).

For $T_{kl}^{(0)}$ we obtain

$$T_{kl}^{(0)} = \frac{\hbar^2}{2m\omega}\int\left[\frac{\partial^2 r_1}{\partial\eta_k^{(1)}\partial\eta_l^{(1)}}\right]\exp\{(i/\hbar)[h_1^{(0)}]\}d_{(3)}\rho^{(1)} + \frac{i}{\hbar m\omega}\int \alpha_{kl}^{(1)}[r_1]\exp\{(i/\hbar)[h_1^{(0)}]\}d_{(3)}\rho^{(1)}$$

$$+\frac{2}{\omega}\int v'\frac{\xi_k^{(2)}+\tfrac{1}{2}(\rho_k^{(1)}+\rho_k^{(2)})}{|\xi^{(2)}+\tfrac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\xi_l^{(2)}[r_2]\exp\{(i/\hbar)[h_2^{(0)}]\}d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}. \quad (6.12)$$

The first term corresponds to the kinetic part of hydrostatic pressure. The second term depends on the coefficient $\alpha_{kl}^{(1)}$ vanishing for $u_k=\omega_k=0$, and is symmetric with respect to the indices k and l. The third term, joined with the intermolecular potential, has not a definite symmetry (provided that $[h_2^{(0)}]$ has a very special structure) and behaves quite similarly to its classical analog, giving in general the coupling between the equation of momentum and that of angular momentum. There may be of course some quantitative differences following from the quantum effects, which exists on the level of Gibbs distributions and which may be modified by the existence of the velocities u_k and ω_k.

$Q_{kl}^{(0)}$ has the form:

$$Q_{kl}^{(0)} = \frac{i}{2m\omega\hbar}\int \epsilon_{kmn}\rho_m^{(1)}\gamma_{kn}^{(1)}[r_1]\exp\{(i/\hbar)[h_1^{(0)}]\}d_{(3)}\rho^{(1)}$$

$$-\frac{1}{2\omega^2}\int \epsilon_{kmn}v'\frac{(\rho_m^{(1)}-\rho_m^{(2)})\xi_n^{(2)}+\rho_m^{(1)}\rho_n^{(2)}}{|\xi^{(2)}+\tfrac{1}{2}(\rho^{(1)}+\rho^{(2)})|}\xi_l^{(2)}\exp\{(i/\hbar)[h_1^{(0)}]\}[r_2]d_{(3)}\rho^{(1)}d_{(3)}\rho^{(2)}d_{(3)}\xi^{(2)}. \quad (6.13)$$

In hydrostatic equilibrium, $Q_{kl}^{(0)}=0$. The quantities $T_{kl}^{(0)}$ and $Q_{kl}^{(0)}$ should be tensors expressible by means of the vectors u_k and ω_k. The parts of these tensors which do not vanish for $u_k=\omega_k=0$ may be called the hydrostatic ones, and the vanishing parts must be called the hydrodynamic parts of the tensors $T_{kl}^{(0)}$ and $Q_{kl}^{(0)}$.

Quite analogous forms may be obtained for the vector $q_k^{(0)}$.