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A note on the physical foundation of the theory of multipole-stresses

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BALANCE equations for linear momentum, angular momentum and energy are derived for the model of a body, consisting of a very large number of molecules, each composed of a number of subparticles. The method for deriving the equations is based on classical statistical mechanics (ensemble theory). Many aspects of the phenomenological theories of micropolar elasticity are confirmed. It appears that the inclusion of ever higher derivatives of the strain gradient in continuum mechanics is set bound to, by the existence of stress fluctuations. It is believed that a generalization of the molecular theory on quantum-mechanical basis is possible. The theory may also be applied to the consideration of a continuous body, composed of a large number of very small grains. The conditions for the possibility of application is ensured if statistical methods may be used.

Równania bilansu dla pędu, momentu pędu i energii wyprowadzono dla modelu ciała składającego się z bardzo dużej ilości cząstek, z których każda złożona jest z pewnej liczby podcząstek. Metoda wyprowadzenia równań oparta jest na klasycznej mechanice statystycznej (teorii zbiorów). Potwierdzono wiele aspektów fenomenologicznych mikropolarnej teorii sprężystości. Okazuje się, że uwzględnianie każdej z wyższych pochodnych gradientu odkształcenia jest uzależnione od istnienia fluktuacji naprężeń. Przyjmuje się, że uogólnienie teorii molekularnej na bazie mechaniki kwantowej jest możliwe. Przedstawiona teoria może być również zastosowana do badania ośrodka ciągłego złożonego z dużej liczby bardzo małych ziaren. Powodzenie zastosowania będzie zapewnione, jeśli skorzysta się z metod statystycznych.

Уравнения баланса для импульса, момента импульса и энергии выведены для модели тела, состоящего из очень большого количества частиц, каждая из которых состоит из некоторого количества подчастиц. Метод вывода уравнений опирается на классической статистической механике (теория множеств). Подтверждено много феноменологических аспектов микрополярной теории упругости. Оказывается, что учет каждой из высших производных градиента деформации зависит от существования напряжений — флуктуаций. Верится, что обобщение молекулярной теории на основе квантовой механики возможно. Настоящая теория может быть тоже применена к исследованию сплошной среды, состоящей из большого количества очень малых зерен. Успех применения будет обеспечен, если используется статистические методы.

1. Introduction

IN this paper we consider the derivation of the equations of multipolar continuum mechanics from the principles of classical statistical mechanics. In particular, we shall derive the equations of continuity, of linear and angular momentum and of energy. The model under discussion is a body, consisting of a very large number of molecules. Each of the molecules, which are mutually identical, is composed of a number of subparticles, i.e. the molecules have internal degrees of freedom. For simplicity we shall not specify the kind of particles e.g. charges, dipoles, electric or magnetic multipoles, but we assume the existence of an interaction potential energy of a very general form.

It appears that many aspects of the phenomenological theories of micropolar elasticity are confirmed. However, many other features of theories, that have been developed during

the last decades, are not verified. For the model under discussion the following important conclusions are arrived at:

a) Multipole-stresses and multipole-moments do exist and expressions are given for these quantities.

b) The motion of any individual molecule can be separated into translational, rotational and deformational parts. From the translations and rotations, the local regular motions may be found by statistical means. Although a corresponding separation for any external micro-deformation might formally be possible, physical theory indicates that such a separation is of little significance. A natural bound is set by the existence of stress-fluctuations.

c) Therefore, for the contributions of the molecules to the linear and angular momentum, they are considered as rigid bodies.

d) Because of c), the forces and moments between arbitrary pairs of multipoles only work in, or are taken with respect to the centres of masses.

e) Thus, while the subparticles are mutually interacting, the origin of multipole-stresses cannot be ascribed to the multipole-distributions inside the individual molecules.

f) The real origin of these stresses and moments is of a statistical nature. In ensemble theory, it is the pair distribution function, which gives rise to contributions by molecules, situated at different places, to those stresses and moments. Effectively they form the multipoles.

g) As a conclusion of f) also multipole-stresses occur between molecules without internal degrees of freedom (point-masses).

h) We will in this paper also introduce multipole-body-forces and moments, but they are believed to be small with respect to the corresponding stresses. This is a consequence of the fact that the external field will be more smooth than the internal field.

i) In the existing phenomenological theories, heat supplies and heat fluxes are introduced, but they are considered independently from the forces. In this theory the total local energy can be divided into the work, performed by the body-forces, stresses and moments in the regular motions, and the heat supply, which is the work performed in the internal irregular motions. Correspondingly the energy flux may be split into the work by stresses and moments and the heat flux. It is obvious that the heat flux consists of a sum of multipole heat fluxes.

While the molecular theory is based on classical mechanics and classical statistical mechanics, it is believed that a generalisation on quantum-mechanical basis is possible.

It is expected that the deviations between the classical theory and the multipole-stress-theory, on this molecular basis, are numerically very small. Therefore it is worth while to look for a model, to which the present theory may be applied, while the deviations from classical theory are possibly somewhat greater. Such a model is provided by a continuous body, consisting of a large number of very small grains. The condition, that this theory may be applied, is ensured if, for the description of the properties of the body, statistical methods can be used, while the forces between the grains can be derived from a potential function. The "molecules" are now the grains and the subparticles are the particles in the grains. While the characteristic length parameter for the grains is considerably greater than the corresponding one in the molecular theory, the derivative of

the pair distribution function is here very small, i.e. the average force on one of the grains exerted by the others is small.

The first who have derived the equations of hydrodynamics by the methods of statistical mechanics are IRVING and KIRKWOOD [1]. This work is generalised to the derivation of the equations of quantum hydrodynamics by IRVING and ZWANZIG [2]. In [3] both papers are included, and in [4] a summary of [1] is presented. KELLER and KELLER [5] have given the first proof that moment-stresses can be found in statistical mechanics. ALBLAS and KUIPERS [6] have extended the theory of KELLER and KELLER for the case of dipolar molecules.

It is the purpose of this paper to provide the physical basis for the theory of generalised media and to obtain formulae, which make possible a numerical estimation of the quantities involved. We shall derive and even generalize the results, obtained by GREEN and RIVLIN [7], in their first paper on the continuum mechanics of multipole-stresses. Green and Rivlin's contributions can be considered to belong to the most general ones in this theory.

Before entering upon the details of the multipole-stress theory we shall make a few remarks concerning stress-fluctuations. According to classical statistical mechanics [8], the following relation exists

$$\overline{(\delta p)^2} = -kT\left(\frac{\partial p}{\partial V}\right)_S, \tag{1.1}$$

where p is the pressure, V the volume, T the absolute temperature, S the entropy and k Boltzmann's constant. The deviation from the average value is denoted by δ, thus δp is the deviation due to fluctuations in the pressure. The bar denotes the average value.

Applying (1.1) to the case of a gas we find

$$\overline{(\delta p)^2} = \frac{kT\varrho c_0^2}{\Delta V}, \tag{1.2}$$

with ϱ the density, c_0 the velocity of sound, calculated from the equilibrium equation of state, while ΔV is the volume-element over which the deviation is measured. If we apply (1.1) to a solid body we find

$$\overline{(\delta p)^2} = \frac{kT\varkappa}{\Delta V}, \tag{1.3}$$

where $\varkappa$ is the adiabatic compressibility. Without distinguishing this from the isothermal compressibility, we have

$$\sqrt{\overline{(\delta p)^2}} = \sqrt{\frac{kTE}{3(1-2\nu)}}\frac{1}{\sqrt{\Delta V}} \approx \frac{1}{5}10^{-6}\frac{1}{l^{3/2}}\ \mathrm{kg/cm^2}, \tag{1.4}$$

for metals at room temperature. From (1.4) it follows that a stress deviation of about 30 kg/cm^2, i.e. 1% of an average yield value, occurs in a cube with the edge $\frac{1}{4}\cdot 10^{-4}$ mm $=$ $= 0.025\mu$.

The basic idea is now the following. For a Cosserat-type medium, the state of deformation is described by displacement-gradients up to a certain order. Dimensional

analysis then shows that the medium is characterised by a number of length parameters, together with more conventional moduli. It is well known that such length parameters give rise to the existence of boundary layers with comparable size, in which the gradient of the stress is considerable. It is obvious that each of the length parameters must be greater than the critical fluctuation parameter. As it must be expected that by increasing the order of differentiation, the corresponding length parameter decreases, a bound is set to the order of the equations. Shortly, continuization of discrete systems is only possible, if the external and internal fields are smooth enough. In that case, higher order derivatives become practically zero above a certain order.

However, in our theory, we shall expand the functions in infinite series and retain all orders. This will only be done for simplicity and the physical meaning of the series, being in fact only finite sums, have to be borne in mind.

2. Kinematics and dynamics of a composite particle

We consider a system of N molecules, each composed of S particles. In a Cartesian coordinate system, the position of the i-th particle of the k-th molecule is given by $\mathbf{R}^{ki}$. The position of the centre of mass of the k-th molecule is $\mathbf{R}^{k}$. Then we define $\mathbf{r}^{ki}$ by (cf. Fig. 1)

$$\mathbf{R}^{ki} = \mathbf{R}^{k} + \mathbf{r}^{ki}. \tag{2.1}$$

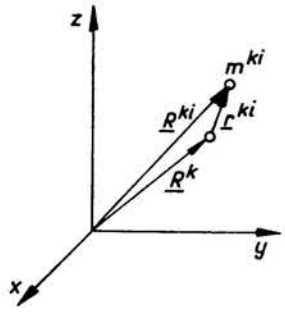

FIG. 1.

If the mass of the particle ki is given by m^{ki}, we have

$$m\mathbf{R}^{k} = \sum_{i} m^{ki}\mathbf{R}^{ki}, \tag{2.2}$$

where

$$m = \sum_{i} m^{ki}. \tag{2.3}$$

From (2.2) follows

$$\sum_{i} m^{ki}\mathbf{r}^{ki} = 0. \tag{2.4}$$

If we differentiate (2.1) with respect to the time, denoted by a dot, we have

$$\dot{\mathbf{R}}^{ki} = \dot{\mathbf{R}}^{k} + \dot{\mathbf{r}}^{ki}. \tag{2.5}$$

Now we write

$$\dot{\mathbf{r}}^{ki} = \boldsymbol{\omega}^{k} \times \mathbf{r}^{ki} + \mathbf{v}^{ki}, \tag{2.6}$$

where $\boldsymbol{\omega}^{k}$ is the local angular velocity of the molecule as a rigid body, while $\mathbf{v}^{ki}$ are the internal relative velocities. We define $\boldsymbol{\omega}^{k}$ in the following way. Introducing the local inertia tensor $J^{k}_{\alpha\beta}$ in the form as it takes in the mechanics of rigid bodies, we write

$$\sum_{i} m^{ki}(\mathbf{r}^{ki} \times \dot{\mathbf{r}}^{ki})_{\alpha} = J^{k}_{\alpha\beta}\omega^{k}_{\beta}, \tag{2.7}$$

and by this equation ω^{k}_{β} is uniquely determined.

If we now split $\dot{\mathbf{r}}^{ki}$ according to (2.6) we find

$$\sum_{i} m^{ki}\mathbf{r}^{ki} \times \mathbf{v}^{ki} = 0. \tag{2.8}$$

Because of (2.4) we further have

$$\sum_{i} m^{ki}\mathbf{v}^{ki} = 0. \tag{2.9}$$

The conditions (2.8) and (2.9) express the fact that the deformational (vibrational) modes of the molecule do not contribute to angular momentum and linear momentum, respectively. For practical calculations this separation of rotation and vibration is not convenient (cf. [9]). But for our purpose, it suffices.

For the kinetic energy we have

$$E^{k} = \sum_{i} \frac{1}{2} m^{ki}(\dot{\mathbf{R}}^{ki})^{2} = \frac{1}{2} m(\dot{\mathbf{R}}^{k})^{2} + \frac{1}{2} J^{k}_{\alpha\beta}\omega^{k}_{\alpha}\omega^{k}_{\beta} + \sum_{i} \frac{1}{2} m^{ki}(\mathbf{v}^{ki})^{2}. \tag{2.10}$$

We now assume Newton's law to hold for any particle. Thus we have

$$m^{ki}\ddot{\mathbf{R}}^{ki} = \mathbf{F}^{ki} + \mathbf{f}^{ki}, \tag{2.11}$$

where $\mathbf{F}^{ki}$ is the external force and $\mathbf{f}^{ki}$ the internal interaction force. If we sum (2.11) over i we find the equation for the motion of the centre of mass

$$m\ddot{\mathbf{R}}^{k} = \mathbf{F}^{k} + \mathbf{f}^{k}, \tag{2.12}$$

with

$$\mathbf{F}^{k} = \sum_{i} \mathbf{F}^{ki}; \quad \mathbf{f}^{k} = \sum_{i} \mathbf{f}^{ki}. \tag{2.13}$$

We also introduce the angular momentum $\mathbf{H}^{k}$ by

$$\mathbf{H}^{k} = \sum_{i} m^{ki}(\mathbf{R}^{ki} \times \dot{\mathbf{R}}^{ki}), \tag{2.14}$$

that can be decomposed into two parts $\mathbf{D}^{k}$ and $\mathbf{d}^{k}$, according to

$$\mathbf{D}^{k} = m(\mathbf{R}^{k} \times \dot{\mathbf{R}}^{k}), \tag{2.15}$$

$$\mathbf{d}^{k} = \sum_{i} m^{ki}(\mathbf{r}^{ki} \times \dot{\mathbf{r}}^{ki}). \tag{2.16}$$

For $\mathbf{d}^k$ we will write

$$d_\alpha^k = J_{\alpha\beta}^k \omega_\beta^k, \tag{2.17}$$

where d_α^k denotes the α-component of $\mathbf{d}^k$.

In (2.17) we have applied the summation convention to the component indices β. This will generally be done. To the numbers k and i, we shall never apply this convention. Differentiating (2.14) with respect to the time, and using (2.11), we find

$$\dot{H}_\alpha^k = \dot{D}_\alpha^k + \dot{d}_\alpha^k = \mathbf{R}^k \times \mathbf{F}^k + \sum_i \mathbf{r}^{ki} \times \mathbf{F}^{ki} + \mathbf{R}^k \times \mathbf{f}^k + \sum_i \mathbf{r}^{ki} \times \mathbf{f}^{ki}. \tag{2.18}$$

3. The distribution functions

One of the most fundamental errors, made in the continuum mechanics of the Cosserat type media, is owing to the fact that molecular quantities are introduced, e.g. the local spin vector, without using statistics. Therefore we shall base our considerations on statistical mechanics; we introduce the N-particle distribution function $f^{(NS)}$ as a function of the parameters

$$f^{(NS)} = f^{(NS)}(\mathbf{R}^1, \mathbf{r}^{11}, \ldots, \mathbf{r}^{1S}, \dot{\mathbf{R}}^1, \dot{\mathbf{r}}^{11}, \ldots, \mathbf{R}^2, \mathbf{r}^{21}, \ldots, \dot{\mathbf{r}}^{NS}, t). \tag{3.1}$$

The probability that the N distinct molecules occupy the volume elements $\mathbf{R}^k$, $d\mathbf{R}^k$ with the velocities in the range $\dot{\mathbf{R}}^k$, $d\dot{\mathbf{R}}^k$ and the corresponding ranges hold for the internal positions and velocities is (cf. [3] and [10])

$$f^{(NS)} \prod_{k=1}^{N} d\mathbf{R}^k d\dot{\mathbf{R}}^k \prod_{i=1}^{S} d\mathbf{r}^{ki} d\dot{\mathbf{r}}^{ki}. \tag{3.2}$$

We also introduce

$$f^{(N)} = \int f^{(NS)} \prod_{i=1}^{S} d\mathbf{r}^{ki} d\dot{\mathbf{r}}^{ki}. \tag{3.3}$$

Especially important are

$$f^{(1)} = \int f^{(N)}(\mathbf{R}^k, \dot{\mathbf{R}}^k, t) \prod_{k=2}^{N} d\mathbf{R}^k d\dot{\mathbf{R}}^k, \tag{3.4}$$

$$n_1 = \int f^{(1)}(\mathbf{R}^1, \dot{\mathbf{R}}^1, t) d\dot{\mathbf{R}}^1, \tag{3.5}$$

$$n_2 = \int f^{(2)}(\mathbf{R}^1, \dot{\mathbf{R}}^1, \mathbf{R}^2, \dot{\mathbf{R}}^2, t) d\dot{\mathbf{R}}^1 d\dot{\mathbf{R}}^2. \tag{3.6}$$

It is possible to consider the $f^{(k)}$'s as probability functions, all normalized to 1. For practical purposes it is better to consider the $f^{(k)}$'s as number densities and to normalize $f^{(1)}$ and n_1 to N, $f^{(2)}$ and n_2 to $N(N-1)$ etc. (cf. [3, 4, 10]).

The function $f^{(NS)}$ satisfies Liouville's equation. By integration we derive

$$\frac{\partial n_2}{\partial t} + \sum_{k=1}^{2} \frac{\partial}{\partial \mathbf{R}^k} (n_2 \bar{\mathbf{v}}^k) = 0, \tag{3.7}$$

with

$$\bar{\mathbf{v}}^k = \frac{1}{n_2}\int f^{(2)}(\mathbf{R}^k, \dot{\mathbf{R}}^k, \mathbf{R}^l, \dot{\mathbf{R}}^l, t)\dot{\mathbf{R}}^k d\dot{\mathbf{R}}^k d\dot{\mathbf{R}}^l. \tag{3.8}$$

The average value $A(\mathbf{R}, t)$ of a microscopic quantity $a(\mathbf{R}, \mathbf{R}^{ki}, \dot{\mathbf{R}}^{ki}, t)$ is defined and denoted by

$$A(\mathbf{R}, t) = \langle a; f\rangle = \int a f^{(N)} d\varphi, \tag{3.9}$$

where φ is an abbreviation for the fluxion space element. There are simple calculation rules for the derivation of $\langle a; f\rangle$. If the quantities a are sums of functions, which depend on the variables pertinent to one or to two molecules only, many of the integrations may be performed and the resulting average values simplify considerably (cf. [11]).

4. Basic definitions

We define:

a) the density ϱ

$$\varrho = \Big\langle \sum_k m\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.1}$$

where $\delta(\mathbf{R}^k - \mathbf{R})$ is Dirac's Delta-function.

(4.1) may be written as

$$\varrho = m\int f^{(1)}(\mathbf{R}^k, \dot{\mathbf{R}}', \mathbf{r}'', \dot{\mathbf{r}}'', t)\cdot\delta(\mathbf{R}^k - \mathbf{R}) d\mathbf{R}^k d\dot{\mathbf{R}}' d\mathbf{r}'' d\dot{\mathbf{r}}'' = mn_1(\mathbf{R}, t); \tag{4.2}$$

b) the local momentum $\varrho\mathbf{v}$

$$\varrho\mathbf{v} = \Big\langle \sum_k m\dot{\mathbf{R}}^k\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.3}$$

for which we may write

$$\varrho\mathbf{v} = m\int \dot{\mathbf{R}}' f^{(1)}(\mathbf{R}, \dot{\mathbf{R}}', t) d\dot{\mathbf{R}}'; \tag{4.4}$$

c) the local internal angular momentum

$$\varrho I_{\alpha\beta}\omega_\beta \equiv J_{\alpha\beta}\omega_\beta = \Big\langle \sum_{k,l} m^{kl}(\mathbf{r}^{ki}\times\dot{\mathbf{r}}^{ki})_\alpha\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.5}$$

that becomes

$$J_{\alpha\beta}\omega_\beta = \int J^k_{\alpha\beta}\omega^k_\beta n_1(\mathbf{R}, \mathbf{r}'', \dot{\mathbf{r}}'', t) d\mathbf{r}'' d\dot{\mathbf{r}}''; \tag{4.6}$$

d) the local angular velocity $\boldsymbol{\omega}$

$$\boldsymbol{\omega} = \frac{\big\langle \sum_k \boldsymbol{\omega}^k\delta(\mathbf{R}^k - \mathbf{R}); f\big\rangle}{n_1(\mathbf{R}, t)}, \tag{4.7}$$

from which we derive

$$\int(\boldsymbol{\omega} - \boldsymbol{\omega}^k) n_1(\mathbf{R}, \mathbf{r}'', \dot{\mathbf{r}}'', t) d\mathbf{r}'' d\dot{\mathbf{r}}'' = 0. \tag{4.8}$$

From (4.6) and (4.7) we derive

$$I_{\alpha\beta} = \frac{\int I^k_{\alpha\beta}\omega^k_\beta n_1(\mathbf{R}, \mathbf{r}'', \dot{\mathbf{r}}'', t)d\mathbf{r}''d\dot{\mathbf{r}}''}{\int \omega^k_\beta n_1(\mathbf{R}, \mathbf{r}'', \dot{\mathbf{r}}'', t)d\mathbf{r}''d\dot{\mathbf{r}}''}, \tag{4.9}$$

where $I^k_{\alpha\beta}$ is introduced as

$$J^k_{\alpha\beta} = mI^k_{\alpha\beta}. \tag{4.10}$$

We further define

e) the local total angular momentum $\varrho\mathbf{H}$

$$\varrho\mathbf{H} = \Big\langle \sum_{k,l} (\mathbf{R}^{kl} \times m^{kl}\dot{\mathbf{R}}^{kl})\,\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.11}$$

f) the local external angular momentum $\varrho\mathbf{D}$

$$\varrho\mathbf{D} = \Big\langle \sum_{k} (\mathbf{R}^k \times m\dot{\mathbf{R}}^k)\,\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle. \tag{4.12}$$

We shall also make use of the following energy definitions:

g) the local kinetic energy

$$\varrho E = \Big\langle \sum_{k,l} \frac{1}{2} m^{kl}(\dot{\mathbf{R}}^{kl})^2 \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle; \tag{4.13}$$

h) the local kinetic part of the internal energy

$$\varrho U^{(k)} = \Big\langle \sum_{k} \Big\{ \frac{1}{2} m(\dot{\mathbf{R}}^k - \mathbf{v})^2 + \frac{1}{2} J^k_{\alpha\beta}\,\omega^k_\alpha(\omega^k_\beta - \omega_\beta) \Big\} \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.14}$$

i) the local potential part of the internal energy

$$\varrho U^{(p)} = \frac{1}{2} \Big\langle \sum_{k,l} u^{kl} \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{4.15}$$

where u^{kl} denotes the interaction energy of the k-th and l-th molecules.

5. Conservation of mass

From (4.1) and (4.4) follows

$$\frac{\partial \varrho}{\partial t} = \Big\langle \sum_k m\dot{R}^{(k)}_\alpha \nabla_{R^k_\alpha} \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle = -\frac{\partial}{\partial R_\alpha} \Big\langle \sum_k m\dot{R}^k_\alpha \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle = -(\varrho v_\alpha)_{,\alpha}, \tag{5.1}$$

from which we derive

$$\dot{\varrho} + \varrho v_{\alpha,\alpha} = 0, \tag{5.2}$$

the well-known equation of mass conservation.

6. The body-forces and moments

The α-component of the body-force, working in an element at $\mathbf{R}$ is

$$K_\alpha = \Big\langle \sum_{k,l} F^{kl}_\alpha \delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle. \tag{6.1}$$

We assume that the external field is a very smooth field. In that case we may write

$$\mathbf{F}^{ki} = \mathbf{F}(\mathbf{R}^{ki}) = \mathbf{F}(\mathbf{R}^k+\mathbf{r}^{ki}) = \sum_{n=0}^{\infty} \frac{1}{n!}(\mathbf{r}^{ki}\cdot\nabla_k)^n \mathbf{F}(\mathbf{R}^k). \tag{6.2}$$

With (6.2), (6.1) becomes

$$K_\alpha = \sum_{n=0}^{\infty} \frac{1}{n!} F_{\alpha,\alpha_1\ldots\alpha_n}(\mathbf{R})\, g^{\alpha_1\ldots\alpha_n}(\mathbf{R}), \tag{6.3}$$

where $g^{\alpha\alpha_1\cdots n}(\mathbf{R})$ has been defined as

$$g^{\alpha_1\ldots\alpha_n}(\mathbf{R}) = \int \varrho_{\alpha_1}\ldots\varrho_{\alpha_n} n_1(\mathbf{R},\boldsymbol{\rho},t)\,d\boldsymbol{\rho}, \tag{6.4}$$

where $\boldsymbol{\rho}$ denotes the internal parameter $\mathbf{r}^{11}$.

For the total moment of the body-forces we find correspondingly

$$\begin{aligned}\mathbf{M} &= \Big\langle \sum_{k,i} (\mathbf{R}^{ki}\times\mathbf{F}^{ki})\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle \\ &= \Big\langle \sum_{k,i} (\mathbf{R}^k\times\mathbf{F}^{ki})\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle + \Big\langle \sum_{k,i} (\mathbf{r}^{ki}\times\mathbf{F}^{ki})\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle.\end{aligned} \tag{6.5}$$

With (6.2) this becomes

$$M_\alpha = e_{\alpha\beta\gamma}R_\beta K_\gamma + e_{\alpha\beta\gamma}\sum_{n=0}^{\infty}\frac{1}{n!}F_{\gamma,\alpha_1\ldots\alpha_n}g^{\beta\alpha_1\ldots\alpha_n}. \tag{6.6}$$

We introduce the moment m_α by

$$m_\alpha = M_\alpha - e_{\alpha\beta\gamma}R_\beta K_\gamma. \tag{6.7}$$

The work performed by the body-forces is given by

$$\begin{aligned}\Big\langle \sum_{k,i}\dot{\mathbf{R}}^{ki}\cdot\mathbf{F}^{ki}\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle &= \Big\langle \sum_k \dot{\mathbf{R}}^k\cdot\mathbf{F}^{ki}\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle \\ &+ \Big\langle \sum_{k,i}\omega^k\cdot(\mathbf{r}^{ki}\times\mathbf{F}^{ki})\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle + \Big\langle \sum_{k,i}\mathbf{v}^{ki}\cdot\mathbf{F}^{ki}\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle.\end{aligned} \tag{6.8}$$

We introduce the heat supply-function per unit time $r^{(k)}$ by

$$r^{(k)} = \Big\langle \sum_{k,i}\mathbf{v}^{ki}\cdot\mathbf{F}^{ki}\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle. \tag{6.9}$$

With (6.2) we may write for the other parts of the work performed

$$\sum_{n=0}^{\infty}\frac{1}{n!}\{F_{\alpha,\alpha_1\ldots\alpha_n}v_\alpha g^{\alpha_1\ldots\alpha_n} + \omega_\alpha e_{\alpha\beta\gamma}F_{\gamma,\alpha_1\ldots\alpha_n}g^{\beta\alpha_1\ldots\alpha_n}\} = v_\alpha K_\alpha + \omega_\alpha m_\alpha. \tag{6.10}$$

The total work performed by the body-forces may be written in the form

$$r^{(k)} + K_\alpha v_\alpha + m_\alpha\omega_\alpha. \tag{6.11}$$

The expression (6.11) is consistent with the model of a rigid body with small deviations. It appears that this model gives rise to contributions in the internal energy, which

contain products of stress- and displacement-gradients of all orders. Therefore it seems appropriate to extend the model for the calculation of the work performed by the body-forces to the model of a deformable molecule. To this end we assume a smooth velocity field and we expand the local translation-energy as follows

$$\mathbf{v}(\mathbf{R}^{ki})\cdot\mathbf{F}(\mathbf{R}^{ki}) = \sum_{n=0}^{\infty}\frac{1}{n!}(\mathbf{r}^{ki}\cdot\nabla_k)^n\{\mathbf{v}(\mathbf{R}^k)\cdot\mathbf{F}(\mathbf{R}^k)\}, \tag{6.12}$$

and correspondingly the energy of rotation. We find for the work in this model

$$K_\alpha v_\alpha + m_\alpha\omega_\alpha + \sum_{n=0}^{\infty}\frac{1}{n!}\{F_\alpha v_{(\alpha,\beta)}\}_{,\alpha_1\ldots\alpha_n}g^{\beta\alpha_1\ldots\alpha_n} + \sum_{n=0}^{\infty}\frac{1}{n!}\{F_\alpha(v_{[\alpha,\beta]}-\omega_{\alpha\beta})\}_{,\alpha_1\ldots\alpha_n}g^{\beta\alpha_1\ldots\alpha_n}. \tag{6.13}$$

In (6.13) $\omega_{\alpha\beta}$ has been defined by

$$\omega_{\alpha\beta} = -\omega_\gamma e_{\gamma\alpha\beta}. \tag{6.14}$$

We note that (6.13) is frame-indifferent. The total work by the body forces may also be written in the form

$$K_\alpha v_\alpha + m_\alpha\omega_\alpha + F_{\alpha\beta}v_{(\alpha,\beta)} + F_{\alpha\beta\gamma}v_{(\alpha,\beta)\gamma} + \ldots + l_{\alpha\beta\gamma}\{v_{[\alpha,\beta]}-\omega_{\alpha\beta}\}_{,\gamma} + \ldots. \tag{6.15}$$

The coefficients in (6.15) are combinations of those in (6.13).

7. The linear momentum

We differentiate (4.3) with respect to the time and obtain

$$\frac{\partial(\varrho v_\alpha)}{\partial t} = \Big\langle\sum_k m\ddot{R}^k_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle + \Big\langle\sum_k m\dot{R}^k_\alpha\dot{R}^k_\beta(\nabla_k\delta(\mathbf{R}^k-\mathbf{R}))_\beta; f\Big\rangle. \tag{7.1}$$

With (2.11) and (2.13) this becomes

$$\frac{\partial(\varrho v_\alpha)}{\partial t} = \Big\langle\sum_{k,i}F^{ki}_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle + \Big\langle\sum_{k,i}f^{ki}_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle - \frac{\partial}{\partial R_\varrho}\Big\langle\sum_k m\dot{R}^k_\alpha\dot{R}^k_\beta\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle. \tag{7.2}$$

We write this in the form

$$\frac{\partial(\varrho v_\alpha)}{\partial t} = K_\alpha - \Big\langle\sum_{\substack{k,i\\l,j}}(\nabla_{ki}u^{kl})_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle - \frac{\partial}{\partial R_\beta}\Big\langle\sum_k m(\dot{R}^k_\alpha-v_\alpha)(\dot{R}^k_\beta-v_\beta)\delta(\mathbf{R}^k-\mathbf{R}); f\Big\rangle - (\varrho v_\alpha v_\beta)_{,\beta}, \tag{7.3}$$

after having used (6.1) and having made the assumption that the internal force $\mathbf{f}^{ki}$ may be derived from an internal potential u^{kl}, according to

$$\mathbf{f}^{ki} = -\sum_{l,j}\nabla_{ki}u^{kl}. \tag{7.4}$$

The internal potential depends on the location of the molecules k and l. For the derivation of (7.3) we further used (4.3).

Introducing the kinetic stress tensor $t^{(k)}_{\alpha\beta}$, according to

$$t^{(k)}_{\alpha\beta} = -\Big\langle \sum_k m(\dot{R}^k_\alpha - v_\alpha)(\dot{R}^k_\beta - v_\beta)\,\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle, \tag{7.5}$$

we may write (7.3), with the aid of (5.1), as follows

$$\varrho \dot{v}_\alpha = K_\alpha + t^{(k)}_{\alpha\beta,\beta} + T_{\alpha\beta,\beta}, \tag{7.6}$$

expressing the balance of linear momentum, with $T_{\alpha\beta}$ the stress tensor, defined by

$$T_{\alpha\beta,\beta} = -\Big\langle \sum_{\substack{k,l \\ i,j}} (\nabla_{ki} u^{kl})_\alpha\,\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle. \tag{7.7}$$

Because

$$\sum_i \nabla_{ki} u^{kl} = -\sum_j \nabla_{lj} u^{kl}, \tag{7.8}$$

we may write (7.7) as

$$T_{\alpha\beta,\beta} = -\frac{1}{2}\Big\langle \sum_{\substack{k,l \\ i,j}} (\nabla_{ki} u^{kl})_\alpha \{\delta(\mathbf{R}^k - \mathbf{R}) - \delta(\mathbf{R}^l - \mathbf{R})\}; f \Big\rangle. \tag{7.9}$$

We expand $\delta(\mathbf{R}^l - \mathbf{R})$ in a series, according to

$$\delta(\mathbf{R}^l - \mathbf{R}) = \delta(\mathbf{R}^l - \mathbf{R}^k + \mathbf{R}^k - \mathbf{R}) = \delta(\mathbf{R}^k - \mathbf{R} + \mathbf{R}^{kl}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{R}^{kl} \cdot \nabla_k)^n \delta(\mathbf{R}^k - \mathbf{R}), \tag{7.10}$$

with

$$\mathbf{R}^{kl} = \mathbf{R}^l - \mathbf{R}^k. \tag{7.11}$$

We shall prove that

$$\sum_i \nabla_{ki} u^{kl} = \nabla_k u^{kl}; \tag{7.12}$$

thus (7.9) may be written as

$$T_{\alpha\beta,\beta} = \sum_{n=1}^{\infty} t_{\alpha\beta_1 \ldots \beta_n, \beta_1 \ldots \beta_n}, \tag{7.13}$$

where $t_{\alpha\beta_1 \ldots \beta_n}$ has been defined by

$$t_{\alpha\beta_1 \ldots \beta_n} = \frac{1}{2} \frac{(-1)^n}{n!} \Big\langle \sum_{k,l} (\nabla_k u^{kl})_\alpha R^{kl}_{\beta_1} \ldots R^{kl}_{\beta_n}\,\delta(\mathbf{R}^k - \mathbf{R}); f \Big\rangle. \tag{7.14}$$

From (7.13) it follows that we have

$$T_{\alpha\beta} = \sum_{n=2}^{\infty} t_{\alpha\beta\beta_2 \ldots \beta_n, \beta_2 \ldots \beta_n} + t_{\alpha\beta}. \tag{7.15}$$

We now enter upon the form of u^{kl}. For a very general case, the case of multipole interactions (cf. [11]), we can derive the expression

$$u^{kl} = \sum_{i,j}\sum_{m,n=0}^{\infty} \frac{1}{m!\,n!}(\mathbf{r}^{ki}\cdot\nabla_k)^m(\mathbf{r}^{lj}\cdot\nabla_l)^n\frac{1}{R}, \tag{7.16}$$

where

$$R = |\mathbf{R}^{kl}| = |\mathbf{R}^l - \mathbf{R}^k|. \tag{7.17}$$

From (7.16) we can see that

$$\sum_i \nabla_{ki}u^{kl} = \sum_i \frac{\partial}{\partial \mathbf{R}^{ki}}u^{kl} = \sum_i \frac{\partial}{\partial \mathbf{r}^{ki}}u^{kl} = \nabla_k u^{kl}. \tag{7.18}$$

We note that it is often advantageous to expand the stress tensor $T_{\alpha\beta}$ according to

$$T_{\alpha\beta} = t_{\alpha\beta} + \sum_{n=1}^{\infty} t_{\alpha\beta\beta_1\ldots\beta_n,\beta_1\ldots\beta_n}. \tag{7.19}$$

In that case $t_{\alpha\beta\beta_1\ldots\beta_n}$ have to be redefined by

$$t_{\alpha\beta\beta_1\ldots\beta_n} = \frac{1}{2}\frac{(-1)^{n+1}}{(n+1)!}\left\langle \sum_{k,l}(\nabla_k u^{kl})_\alpha R^{kl}_\beta R^{kl}_{\beta_1}\ldots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R}); f\right\rangle. \tag{7.20}$$

In terms of the pair distribution function, (7.20) becomes

$$t_{\alpha\beta\beta_1\ldots\beta_n} = \frac{1}{2}\frac{(-1)^n}{(n+1)!}\int\{\nabla_\varrho u(\mathbf{R},\boldsymbol{\rho},\mathbf{r}^{11},\mathbf{r}^{21})\}_\alpha \varrho_\beta\varrho_{\beta_1}\ldots\varrho_{\beta_n} \cdot n_2(\mathbf{R},\mathbf{R}+\boldsymbol{\rho},\mathbf{r}^{11},\mathbf{r}^{21})\,d\boldsymbol{\rho}\,d\mathbf{r}^{11}d\mathbf{r}^{21}. \tag{7.21}$$

Because of symmetry we see that

$$t_{\alpha\beta\beta_1\ldots\beta_n} = 0 \quad \text{for} \quad n = 1, 3, 5, \ldots. \tag{7.22}$$

8. The angular momentum

It follows directly from the definitions (4.11), (4.12) and (4.5) that the following relation exists

$$\varrho H_\alpha = \varrho D_\alpha + \varrho I_{\alpha\beta}\omega_\beta. \tag{8.1}$$

By differentiating (4.11) with respect to the time, we obtain

$$\frac{\partial(\varrho H_\alpha)}{\partial t} = \left\langle \sum_{k,i}(\mathbf{R}^{ki}\times\mathbf{F}^{ki})_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\right\rangle - \left\langle \sum_{k,l}(\mathbf{R}^{ki}\times\nabla_{ki}u^{ki})_\alpha\delta(\mathbf{R}^k-\mathbf{R}); f\right\rangle - \frac{\partial}{\partial R_\beta}\left\langle \sum_{\substack{k,l\\i,j}}(\mathbf{R}^{ki}\times m^{ki}\dot{\mathbf{R}}^{ki})_\alpha\dot{R}^k_\beta\delta(\mathbf{R}^k-\mathbf{R}); f\right\rangle, \tag{8.2}$$

where we have used (2.12) and (2.13).

The first term on the right-hand side of (8.2) is, according to (6.5), equal to M_α, for the second term we write

$$-\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{R}^{ki}\times\nabla_{ki}u^{kl})_\alpha[\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})];\, f\Big\rangle, \tag{8.3}$$

while the third term is written as

$$-(\varrho H_\alpha v_\beta)_{,\beta}-\frac{\partial}{\partial R_\beta}\Big\langle \sum_{k,i} (\mathbf{R}^{ki}\times m^{ki}\dot{\mathbf{R}}^{ki})_\alpha(\dot{R}^k_\beta - v_\beta)\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle. \tag{8.4}$$

The expression (8.3) is based on the fact that we have

$$\sum_j (\mathbf{R}^{ki}\times\nabla_{ki}u^{kl})+\sum_i (\mathbf{R}^{lj}\times\nabla_{lj}u^{kl}) = 0, \tag{8.5}$$

an equation that holds because the sum of the moments of the internal forces with respect to the fixed origin is equal to zero.

We take the several terms together and find

$$\begin{aligned}\varrho\dot{H}_\alpha = M_\alpha &-\frac{1}{2}\Big\langle \sum_{k,l} (\mathbf{R}^k\times\nabla_k u^{kl})_\alpha[\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})];\, f\Big\rangle\\ &-\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})_\alpha[\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})];\, f\Big\rangle\\ &-\Big\{\Big\langle \sum_k (\mathbf{R}^k\times m\dot{\mathbf{R}}^k)_\alpha(\dot{R}^k_\beta - v_\beta)\,\delta(\mathbf{R}^k-\mathbf{R});f\Big\rangle\Big\}_{,\beta}\\ &-\Big\{\Big\langle \sum_{k,i} (\mathbf{r}^{ki}\times m^{ki}\dot{\mathbf{r}}^{ki})_\alpha(\dot{R}^k_\beta - v_\beta)\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle\Big\}_{,\beta}.\end{aligned} \tag{8.6}$$

Introducing into this equation the expression (7.10), rearranging the terms and using (7.14), we obtain

$$\varrho\dot{H}_\alpha = M_\alpha + e_{\alpha\beta\gamma}\sum_{n=1}^{\infty}(R_\beta t_{\gamma\beta_1\ldots\beta_n})_{,\beta_1\ldots\beta_n}+M_{\alpha\beta,\beta}+e_{\alpha\beta\gamma}R_\beta t^{(k)}_{\gamma\delta,\delta}+m^{(k)}_{\alpha\beta,\beta}, \tag{8.7}$$

with the definitions

$$M_{\alpha\beta,\beta} = -\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})_\alpha\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};\, f\Big\rangle, \tag{8.8}$$

and

$$m^{(k)}_{\alpha\beta} = -\Big\langle \sum_{k,i} (\mathbf{r}^{ki}\times m^{ki}\dot{\mathbf{r}}^{ki})_\alpha(\dot{R}^k_\beta - v_\beta)\,\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle. \tag{8.9}$$

As a consequence of (2.7) we find

$$m^{(k)}_{\alpha\beta} = 0. \tag{8.10}$$

For $M_{\alpha\beta,\beta}$ we have

$$M_{\alpha\beta,\beta} = \sum_{n=1}^{\infty} m_{\alpha\beta_1\ldots\beta_n,\beta_1\ldots\beta_n}, \tag{8.11}$$

with

$$m_{\alpha\beta_1\ldots\beta_n} = \frac{1}{2}\frac{(-1)^n}{n!}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})_\alpha R^{kl}_{\beta_1}\ldots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R});\, f\Big\rangle. \tag{8.12}$$

We now consider $\varrho\dot{D}_\alpha$. Similarly as we have obtained the equation for $\varrho\dot{H}_\alpha$, we get

$$\varrho\dot{D}_\alpha = (\mathbf{R}\times\mathbf{K})_\alpha + e_{\alpha\beta\gamma}R_\beta t^{(k)}_{\gamma\delta,\delta} + e_{\alpha\beta\gamma}R_\beta T_{\gamma\delta,\delta}. \tag{8.13}$$

This equation could directly be found from (7.6) by multiplying it with the vector $\mathbf{R}$. It does not give any new information. With (8.1), (8.7), (8.13) and (6.7) we find

$$\dot{\overline{\varrho(I_{\alpha\beta}\omega_\beta)}} = m_\alpha + M_{\alpha\beta,\beta} + e_{\alpha\beta\gamma}t_{[\gamma\beta]} + e_{\alpha\beta\gamma}\sum_{n=1}^{\infty}(n+1)t_{[\gamma\beta]\beta_1\ldots,\beta_n,\beta_1\ldots\beta_n}. \tag{8.14}$$

There is a relationship between $m_{\alpha\beta_1\ldots\beta_n}$, defined in (8.12) and $t_{\alpha\beta_1\ldots\beta_n}$, according to (7.14).

The potential energy u^{kl} may be expressed as

$$u^{kl} = u(\mathbf{R}^{kl}, \mathbf{R}^{ki}, \mathbf{R}^{lj}), \tag{8.15}$$

but also as

$$u^{kl} = u(\mathbf{R}^{kl}, \mathbf{r}^{ki}, \mathbf{r}^{lj}). \tag{8.16}$$

Because (8.16) has to be frame-indifferent we have

$$R^{kl}_{[\alpha}\frac{\partial u}{\partial R^{kl}_{\beta]}} + \sum_i r^{ki}_{[\alpha}\frac{\partial u}{\partial r^{ki}_{\beta]}} + \sum_j r^{lj}_{[\alpha}\frac{\partial u}{\partial r^{lj}_{\beta]}} = 0. \tag{8.17}$$

This equation may also be obtained from (8.5) if we make use of

$$\frac{\partial u}{\partial \mathbf{R}^{ki}} = \frac{\partial u}{\partial \mathbf{r}^{ki}}. \tag{8.18}$$

Introducing (8.17) and (8.18) into (8.12) we find

$$\begin{aligned} m_{\alpha\beta_1\ldots\beta_n} &= \frac{1}{4}\frac{(-1)^n}{n!}\int e_{\alpha\beta\gamma}[r^{ki}_\beta(\nabla_{ki}u^{kl})_\gamma + r^{lj}_\beta(\nabla_{lj}u^{ki})_\gamma] \\ &\qquad \times \varrho_{\beta_1}\ldots\varrho_{\beta_n}n_2(\mathbf{R}, \mathbf{R}+\boldsymbol{\rho}, \mathbf{r}^{11}, \ldots, \mathbf{r}^{2S})\,d\boldsymbol{\rho}\,d\mathbf{r}^{11}\ldots d\mathbf{r}^{2S} \\ &= -\frac{1}{4}\frac{(-1)^n}{n!}e_{\alpha\beta\gamma}\int \varrho_\beta(\nabla_{kl}u^{kl})_\gamma\varrho_{\beta_1}\ldots\varrho_{\beta_n}n_2(\mathbf{R}, \mathbf{R}+\boldsymbol{\rho})\,d\boldsymbol{\rho} = -\frac{1}{2}(n+1)e_{\alpha\beta\gamma}t_{\gamma\beta\beta_1\ldots\beta_n}. \end{aligned} \tag{8.19}$$

From (8.19) and (7.22) it follows that

$$m_{\alpha\beta_1\ldots\beta_n} = 0 \quad \text{for} \quad n = 1, 3, 5, \ldots. \tag{8.20}$$

With (8.19) we may simplify (8.14). It turns out to become

$$\dot{\overline{\varrho I_{\alpha\beta}\omega_\beta}} = m_\alpha - M_{\alpha\beta,\beta} + e_{\alpha\beta\gamma}t_{[\gamma\beta]}. \tag{8.21}$$

We still can write (8.21) in another form, eliminating $M_{\alpha\beta}$. This form is

$$\dot{\overline{\varrho I_{\alpha\beta}\omega_\beta}} = m_\alpha + e_{\alpha\beta\gamma}T_{[\gamma\beta]} + \frac{1}{2}\sum_{n=1}^{\infty}e_{\alpha\beta\gamma}(n-1)t_{[\gamma\beta]\beta_1\ldots\beta_n,\beta_1\ldots\beta_n}. \tag{8.22}$$

The Eqs. (8.14), (8.21) and (8.22) express the balance of internal angular momentum.

9. The energy

From the definitions (4.13), (4.14) and (4.5) we obtain

$$\varrho E = \varrho U^{(k)} + \frac{1}{2}\varrho v^2 + \frac{1}{2}\varrho I_{\alpha\beta}\omega_\alpha\omega_\beta . \tag{9.1}$$

It may easily be proved that

$$\dot{I}_{\alpha\beta}\omega_\alpha\omega_\beta = 0 , \tag{9.2}$$

from which follows

$$\overline{\frac{1}{2} I_{\alpha\beta}\omega_\alpha\omega_\beta}^{\cdot} = \overline{I_{\alpha\beta}\omega_\beta}^{\cdot}\omega_\alpha . \tag{9.3}$$

By differentiating (4.13) we find

$$\varrho\dot{E} = -\frac{\partial}{\partial R_\alpha}\Big\langle \sum_{k,i} m^{ki}(\dot{\mathbf{R}}^{ki})^2(\dot{R}^k_\alpha - v_\alpha)\,\delta(\mathbf{R}^k - \mathbf{R}); f\Big\rangle + r^{(k)} + K_\alpha v_\alpha + m_\alpha\omega_\alpha - \Big\langle \sum_{\substack{k,l\\ i,j}} (\dot{\mathbf{R}}^{ki}\cdot\nabla_{ki}u^{kl})\,\delta(\mathbf{R}^k - \mathbf{R}); f\Big\rangle , \tag{9.4}$$

where the result (6.11) has been applied.

Next, we differentiate (4.15) with respect to the time. This yields

$$\varrho\dot{U}^{(p)} = \frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\dot{\mathbf{R}}^{ki}\cdot\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k - \mathbf{R}) + \delta(\mathbf{R}^l - \mathbf{R})\}; f\Big\rangle - \frac{\partial}{\partial R_\alpha}\frac{1}{2}\Big\langle \sum_{k,l} u^{kl}(\dot{R}^k_\alpha - v_\alpha)\,\delta(\mathbf{R}^k - \mathbf{R}); f\Big\rangle . \tag{9.5}$$

Introducing

$$U = U^{(k)} + U^{(p)} \tag{9.6}$$

and taking (9.4) and (9.5) together, we find

$$\varrho(\dot{U} + v_\alpha\dot{v}_\alpha + I_{\alpha\beta}\dot{\omega}_\beta\omega_\alpha) = (t^{(k)}_{\alpha\beta}v_\beta)_{,\alpha} - q^{(k)}_{\alpha,\alpha} + r^{(k)} + K_\alpha v_\alpha + m_\alpha\omega_\alpha - q^{(p_1)}_{\alpha,\alpha} - \frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\dot{\mathbf{R}}^{ki}\cdot\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k - \mathbf{R}) - \delta(\mathbf{R}^l - \mathbf{R})\}; f\Big\rangle , \tag{9.7}$$

where the heat fluxes

$$q^{(k)}_\alpha = +\frac{1}{2}\Big\langle \sum_k m(\dot{\mathbf{R}}^k - \mathbf{v})^2(\dot{R}^k_\alpha - v_\alpha)\,\delta(\mathbf{R}^k - \mathbf{R}); f\Big\rangle \tag{9.8}$$

and

$$q^{(p_1)} = +\frac{1}{2}\Big\langle \sum_{k,l} u^{kl}(\dot{R}^k_\alpha - v_\alpha)\,\delta(\mathbf{R}^k - \mathbf{R}); f\Big\rangle \tag{9.9}$$

are introduced. The last term on the right-hand side of (9.7) is developed according to

$$(9.10)\quad -\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\dot{R}^{ki}\cdot\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle$$

$$= -\frac{1}{2}\Big\langle \sum_{k,l} (\dot{\mathbf{R}}^k\cdot\nabla_k u^{kl})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle$$

$$-\frac{1}{2}\Big\langle \sum_{k,l} \boldsymbol{\omega}^k\cdot(\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle$$

$$-\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{v}^{ki}\cdot\nabla_{ki}u^{ki})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle.$$

The first term on the right-hand side of (9.10) is equal to

$$(9.11)\quad -\frac{1}{2}\Big\langle \sum_{k,l} (\dot{\mathbf{R}}^k-\mathbf{v})\cdot\nabla_k u^{kl}\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle + T_{\alpha\beta,\beta}v_\alpha,$$

because of (7.9). The second term in (9.10) will be rewritten in the form

$$(9.12)\quad -\frac{1}{2}\Big\langle \sum_{k,l} (\boldsymbol{\omega}^k-\boldsymbol{\omega})\cdot(\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle + M_{\alpha\beta,\beta}\omega_\alpha,$$

as a consequence of (8.8). We introduce the heat production $r^{(p)}$ per unit time as

$$(9.13)\quad r^{(p)} = -\frac{1}{2}\Big\langle \sum_{\substack{k,l\\ i,j}} (\mathbf{v}^{ki}\cdot\nabla_{ki}u^{kl})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle,$$

and expand the factors in (9.11) and (9.12) according to (7.10). We obtain

$$(9.14)\quad -\frac{1}{2}\Big\langle \sum_{k,l} (\dot{\mathbf{R}}^k-\mathbf{v})\cdot\nabla_k u^{kl}\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle$$

$$= \frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial R_{\beta_1}\dots\partial R_{\beta_n}}\Big\langle \sum_{k,l} (\dot{\mathbf{R}}^k-\mathbf{v})\cdot\nabla_k u^{kl}R^{kl}_{\beta_1}\dots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R});f\Big\rangle$$

$$+\sum_{n=1}^{\infty}{}'(v_\alpha t_{\alpha\beta_1\dots\beta_n})_{,\beta_1\dots\beta_n},$$

where the prime denotes that the term $v_\alpha t_{\alpha\beta_1\dots\beta_n,\beta_1\dots\beta_n}$ must be omitted. Correspondingly we find for the first term in (9.12)

$$(9.15)\quad -\frac{1}{2}\Big\langle \sum_{k,l} (\boldsymbol{\omega}^k-\boldsymbol{\omega})\cdot(\mathbf{r}^{ki}\times\nabla_{ki}u^{ki})\{\delta(\mathbf{R}^k-\mathbf{R})-\delta(\mathbf{R}^l-\mathbf{R})\};f\Big\rangle$$

$$= \frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\partial^n}{\partial R_{\beta_1}\dots\partial R_{\beta_n}}\Big\langle \sum_{\substack{k,l\\ i,j}} (\boldsymbol{\omega}^k-\boldsymbol{\omega})\,(\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})R^{kl}_{\beta_1}\dots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R});f\Big\rangle$$

$$+\sum_{n=1}^{\infty}{}'(\omega_\alpha m_{\alpha\beta_1\dots\beta_n})_{,\beta_1\dots\beta_n}.$$

The first term on the right-hand side of (9.14) is a heat flux term, just like the corresponding term in (9.15). We define

$$q^{(p_2)}_{\alpha,\alpha} = -\frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\Big\{\Big\langle \sum_{k,l}(\dot{\mathbf{R}}^k-\mathbf{v})\cdot\nabla_k u^{kl}\cdot R^{kl}_{\beta_1}\dots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R});f\Big\rangle\Big\}_{,\beta_1\dots\beta_n}, \tag{9.16}$$

and

$$q^{(p_3)}_{\alpha,\alpha} = -\frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\Big[\Big\langle \sum_{k,l}(\boldsymbol{\omega}^k-\boldsymbol{\omega})\cdot(\mathbf{r}^{ki}\times\nabla_{ki}u^{kl})R^{kl}_{\beta_1}\dots R^{kl}_{\beta_n}\delta(\mathbf{R}^k-\mathbf{R});f\Big\rangle\Big]_{,\beta_1\dots\beta_n}. \tag{9.17}$$

We now take the Eqs. (9.7), (9.10), (9.11), (9.12), (9.14) and (9.15) together and simplify the result with the aid of (7.6) and (8.14). We obtain

$$\begin{aligned}\varrho\dot{U} = {} & r-Q_{\alpha,\alpha}+t^{(k)}_{\alpha\beta}v_{\alpha,\beta}+t_{(\alpha\beta)}v_{(\alpha,\beta)}+t_{[\alpha\beta]}\{v_{[\alpha,\beta]}-\omega_{\alpha\beta}\}\\ & +\sum_{n=1}^{\infty}(n+1)\{v_{(\alpha,\beta)}t_{(\alpha\beta)\beta_1\dots\beta_n}\}_{,\beta_1\dots\beta_n}+\sum_{n=1}^{\infty}(n+1)\{[v_{[\alpha,\beta]}-\omega_{\alpha\beta}]t_{[\alpha\beta]\beta_1\dots\beta_n}\}_{,\beta_1\dots\beta_n},\end{aligned} \tag{9.18}$$

the balance equation of internal energy, with the definitions

$$r = r^{(k)}+r^{(p)}, \tag{9.19}$$

$$Q_\alpha = q^{(k)}_\alpha+q^{(p_1)}_\alpha+q^{(p_2)}_\alpha+q^{(p_3)}_\alpha. \tag{9.20}$$

Note that the heat flux is composed of an infinite number of multipole heat fluxes.

The Eq. (9.18), which has been derived by means of the methods of statistical mechanics, is a slight generalization of the energy equation, postulated by GREEN and RIVLIN (cf. [7]).

We now introduce the entropy according to the Clausius-Duhem inequality

$$\int_V\Big[\varrho T\dot{S}-r+Q_{\alpha,\alpha}-\frac{Q_\alpha T_{,\alpha}}{T}\Big]dV\geqslant 0, \tag{9.21}$$

where the integration has been taken over an arbitrary part of the body with volume V. In (9.21) S is the entropy per unit mass and T the absolute temperature. Eliminating $r-Q_{\alpha,\alpha}$ from (9.21) and the integrated equation (9.18) and introducing Helmholtz free energy ψ by

$$\psi = U-TS, \tag{9.22}$$

we obtain

$$\begin{aligned}\int_V\Big[& \varrho\dot{\psi}+\varrho S\dot{T}-t^{(k)}_{\alpha\beta}v_{(\alpha,\beta)}-t_{(\alpha\beta)}v_{(\alpha,\beta)}-t_{[\alpha\beta]}\{v_{[\alpha,\beta]}-\omega_{\alpha\beta}\}-\sum_{n=1}^{\infty}(n+1)\\ & \times\{v_{(\alpha,\beta)}t_{(\alpha\beta)\beta_1\dots\beta_n}\}_{,\beta_1\dots\beta_n}-\sum_{n=1}^{\infty}(n+1)\{[v_{[\alpha,\beta]}-\omega_{\alpha\beta}]t_{[\alpha\beta]\beta_1\dots\beta_n}\}_{,\beta_1\dots\beta_n}+\frac{Q_\alpha T_{,\alpha}}{T}\Big]dV\leqslant 0.\end{aligned} \tag{9.23}$$

A method to derive from the inequality (9.23) a set of constitutive equations is well known. In this paper we shall not enter upon it. The discussion of (9.18) and (9.23) is similar to the corresponding one in reference [7].

10. The constitutive equations

The molecular theory not only enables us to derive the balance equations, with this theory we may also find the constitutive equations. In this chapter we shall give some expressions for a few stresses, in terms of the displacement and rotation gradients. We shall limit the discussion to the linear case, and we shall also confine ourselves to the lowest order terms.

We start with the formula (7.21) for $t_{\alpha\beta}$

$$t_{\alpha\beta} = \frac{1}{2}\int (\nabla_\varrho u)_\alpha \varrho_\beta n_2(\mathbf{R}, \mathbf{R}+\boldsymbol{\rho}, \mathbf{r}^{11}, \ldots, \mathbf{r}^{2S}, t)\, d\boldsymbol{\rho}\, d\mathbf{r}^{11}, \ldots, d\mathbf{r}^{2S}. \tag{10.1}$$

The material derivative of (10.1) is

$$\dot{t}_{\alpha\beta} = \frac{1}{2}\int (\nabla_\varrho u)_\alpha \varrho_\beta \dot{n}_2\, d\boldsymbol{\rho}\, d\mathbf{r}^{11} \ldots d\mathbf{r}^{2S}. \tag{10.2}$$

For n_2, the following equation approximately holds (cf. [6])

$$\frac{\partial n_2}{\partial t} + \frac{\partial (n_2 v_\alpha^1)}{\partial R_\alpha^1} + \frac{\partial (n_2 v_\alpha^2)}{\partial R_\alpha^2} + \sum_i \frac{\partial n_2}{\partial r_\alpha^{1i}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{1i} + \sum_j \frac{\partial n_2}{\partial r_\alpha^{2j}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{2j} = 0, \tag{10.3}$$

where R_α^1 and v_α^1 refer to the α-components of position and velocity of the first particle, while a corresponding definition holds for R_α^2 and v_α^2. The Eq. (10.3) is a generalization, but also a simplification of the exact Eq. (3.7).

We first transform the function $n_2(\mathbf{R}^1, \mathbf{R}^2, \mathbf{r}^{11}, \ldots, \mathbf{r}^{2S}, t)$ into the function $n_2(\mathbf{R}, \mathbf{R}+\boldsymbol{\rho}, \mathbf{r}^{11}, \ldots, \mathbf{r}^{2S}, t)$, according to

$$\mathbf{R} = \mathbf{R}^1, \boldsymbol{\rho} = \mathbf{R}^2 - \mathbf{R}^1. \tag{10.4}$$

We obtain

$$\frac{\partial n_2}{\partial t} + n_2 v_{\alpha,\alpha}^1 + \frac{\partial n_2}{\partial R_\alpha} v_\alpha^1 - \frac{\partial n_2}{\partial \varrho_\alpha} v_\alpha^1 + n_2 v_{\alpha,\alpha}^2 + \frac{\partial n_2}{\partial \varrho_\alpha} v_\alpha^2 + \sum_i \frac{\partial n_2}{\partial r_\alpha^{1i}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{1i} + \sum_j \frac{\partial n_2}{\partial r_\alpha^{2j}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{2j} = 0. \tag{10.5}$$

Writing

$$v_\alpha^1 = v_\alpha; \quad v_\alpha^2 = v_\alpha(\mathbf{R}+\boldsymbol{\rho}) = v_\alpha + v_{\alpha,\beta}\varrho_\beta, \tag{10.6}$$

and approximating to the first two terms and lower derivatives, we have

$$\dot{n}_2 = -2n_2 v_{\alpha,\alpha} - \frac{\partial n_2}{\partial \varrho_\alpha}\varrho_\beta v_{\alpha,\beta} - \sum_i \frac{\partial n_2}{\partial r_\alpha^{1i}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{1i} - \sum_j \frac{\partial n_2}{\partial r_\alpha^{2j}} e_{\alpha\beta\gamma}\omega_\beta r_\gamma^{2j}. \tag{10.7}$$

Now the function n_2 has to be frame-indifferent for fixed $\mathbf{R}$, e.g. it satisfies

$$\frac{\partial n_2}{\partial \varrho_{[\alpha}}\varrho_{\beta]} + \sum_i \frac{\partial n_2}{\partial r_{[\alpha}^{1i}} r_{\beta]}^{1i} + \sum_j \frac{\partial n_2}{\partial r_{[\alpha}^{2j}} r_{\beta]}^{2j} = 0. \tag{10.8}$$

With (10.8), (10.7) becomes

$$\dot{n}_2 = -2n_2 v_{\alpha,\alpha} - \frac{\partial n_2}{\partial \varrho_{(\alpha}}\varrho_{\beta)} v_{(\alpha,\beta)} - \frac{\partial n_2}{\partial \varrho_{[\alpha}}\varrho_{\beta]}\{v_{[\alpha,\beta]} - \omega_{\alpha\beta}\}. \tag{10.9}$$

Introducing (10.9) into (10.2) and integrating over $\mathbf{r}^{11}, \ldots, \mathbf{r}^{2S}$, we find

$$\dot{t}_{\alpha\beta} = \frac{1}{2}\int (\nabla_\varrho u)_\alpha \varrho_\beta \left\{ -2n_2 v_{k,k} - \frac{\partial n_2}{\partial \varrho_{(\alpha}} \varrho_{l)} v_{(k,l)} - \frac{\partial n_2}{\partial \varrho_{[k}} \varrho_{l]} [v_{[k,l]} - \omega_{kl}] \right\} d\boldsymbol{\rho}. \tag{10.10}$$

This expression may be written as

$$\dot{t}_{\alpha\beta} = -2t_{\alpha\beta} v_{k,k} - \frac{1}{2} v_{(k,l)} \int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \frac{\partial n_2}{\partial \varrho_{(k}} \varrho_{l)} d\boldsymbol{\rho} - \frac{1}{2} (v_{[k,l]} - \omega_{kl}) \int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \frac{\partial n_2}{\partial \varrho_{[k}} \varrho_{l]} d\boldsymbol{\rho}. \tag{10.11}$$

If on the stress-free state a small displacement-field $\mathbf{v}\Delta t$ and a small rotation field $\boldsymbol{\omega}\Delta t$ are superposed we have, with

$$\Delta t_{\alpha\beta} = \dot{t}_{\alpha\beta} \Delta t, \quad \mathbf{u} = \mathbf{v}\Delta t, \quad \boldsymbol{\varphi} = \boldsymbol{\omega}\Delta t, \tag{10.12}$$

where Δt is the small time during which the loading takes place,

$$\Delta t_{\alpha\beta} = -\frac{1}{2} u_{(k,l)} \int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \frac{\partial n_2}{\partial \varrho_{(k}} \varrho_{l)} d\boldsymbol{\rho} - \frac{1}{2} [u_{[k,l]} - \varphi_{kl}] \int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \frac{\partial n_2}{\partial \varrho_{[k}} \varrho_{l]} d\boldsymbol{\rho}. \tag{10.13}$$

The integrals are the coefficients of elasticity.

We now consider the stress $t_{[\alpha\beta]\beta_1\beta_2,\beta_2}$, being the main term of the moment-stress tensor. We have

$$\Delta t_{[\alpha\beta]\beta_1\beta_2,\beta_2} = -\frac{1}{12} u_{(k,l)\beta_2} \int \frac{\partial u}{\partial \varrho_{[\alpha}} \varrho_{\beta]} \varrho_{\beta_1} \varrho_{\beta_2} \frac{\partial n_2}{\partial \varrho_{(k}} \varrho_{l)} d\boldsymbol{\rho} - \frac{1}{12} [u_{[k,l]} - \varphi_{kl}]_{,\beta_2} \int \frac{\partial u}{\partial \varrho_{[\alpha}} \varrho_{\beta]} \varrho_{\beta_1} \varrho_{\beta_2} \frac{\partial n_2}{\partial \varrho_{[k}} \varrho_{l]} d\boldsymbol{\rho}, \tag{10.14}$$

in the stress free state, if n_2 does not depend on $\mathbf{R}$. Explicit expressions may be found, if we introduce into (10.13) and (10.14) formulae for u and for n_2.

11. Conclusions

One of the most important questions refers to the order of magnitude of the moment-stress tensor, compared with the stress-tensor. In order to answer this question, we need data concerning the pair distribution function n_2. The quantitative theory of this function for fluids is extremely complicated (cf. [4]), but it is rather easy to give some rough estimations. If we introduce for a fluid the function $g(\boldsymbol{\rho})$, according to

$$n_2 = \varrho^2 g(\boldsymbol{\rho}), \tag{11.1}$$

it is obvious that we have

$$g(0) = 0, \quad g(\infty) = 1. \tag{11.2}$$

Anywhere between 0 and ∞ the g-function of a fluid is very steep and therefore we approximate qualitatively

$$\left(\frac{\partial g}{\partial \varrho}\right)_{\varrho=a} = \text{const}\, \delta(|\boldsymbol{\rho} - \mathbf{a}|). \tag{11.3}$$

Comparing the integrals

$$\int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \frac{\partial n_2}{\partial \varrho_k} \varrho_l d\boldsymbol{\rho} \quad \text{with} \quad \int \frac{\partial u}{\partial \varrho_\alpha} \varrho_\beta \varrho_{\beta_1} \varrho_{\beta_2} \frac{\partial n_2}{\partial \varrho_k} \varrho_l d\boldsymbol{\rho},$$

we see that the ratio is $0(a^2)$.

For a crystalline body, the situation is quite different. Here n_2 is a periodic function and g may be approximated by a series of step functions. The derivative of g with respect to ϱ consists of positive and negative δ-functions. Altogether it appears that in the molecular theory, both of fluids and crystalline bodies, the ratio of the dominant integrals will be very small. Note that a is of the order of a molecular dimension. Thus the effects can be expected to be negligible.

However, for a body consisting of a large number of grains, the corresponding parameter a becomes of the order of the grain dimension. A lower bound for this dimension is given in the introduction. We note that the grains must not be too large, because then the statistical theory cannot be applied and, what is more important, the mutual forces between the grains are not derivable from a potential function. The conclusion is again that the ratio of the integrals will be small.

If the body consists of large grains, we have to deal with the theory of inhomogeneous elasticity.

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