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Balance Equations for Micromorphic Materials

W. Oevel[1] and J. Schröter[1]

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The balance laws for micromorphic continua of degree 1 are derived by means of classical statistical mechanics. The equations derived by Eringen *et al.* [*Continuum Physics*, Vol. IV (Academic, New York, 1976)] are obtained in a slightly generalized form. Explicit expressions for the stress, the couple stress, the spin production, and the heat flux are given in terms of microscopical variables.

KEY WORDS: Balance laws; materials with internal degrees of freedom; stress; spin; couple stress.

1. INTRODUCTION

In this paper we consider materials which are composed of deformable molecules. Such materials are called micromorphic. Their theory was developed about 15 years ago using arguments of phenomenological thermodynamics (cf. Eringen[1]). For the special case of a micromorphic continuum of degree 1 the following quantities are used to define the macroscopical state of the continuum: the mass density ρ, the field of microinertia $\rho \underline{i}$, the local momentum $\rho \underline{v}$, the (generalized) spin density $\rho \underline{\sigma}$, and the internal energy ρ. $\rho \underline{\sigma}$ is called generalized spin, because its antisymmetrical part gives the internal angular momentum of the microcontinua that build up the material, and its symmetrical part gives information about the deformation of the microcontinua.

For these fields the following balance laws were derived (cf. Eringen[1]):

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{1.1}$$

$$\frac{\partial}{\partial t} (\rho \underline{i}) + \nabla \cdot (\mathbf{v} \otimes \rho \underline{i}) = \rho \underline{i} \cdot \underline{\nu} + \rho (\underline{i} \cdot \underline{\nu})^T \tag{1.2}$$

[1] AG Theoretische Physik, Universität Paderborn, 479 Paderborn, West Germany.

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$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\mathbf{v} \otimes \rho \mathbf{v} - \underline{t}) = \mathbf{f} \tag{1.3}$$

$$\frac{\partial}{\partial t}(\rho \underline{\sigma}) + \nabla \cdot (\mathbf{v} \otimes \rho \underline{\sigma} + \underline{\mu}) = \underline{\nu} \cdot \rho \underline{i} \cdot \underline{\nu}^T + \underline{t} - \underline{s} + \underline{l} \tag{1.4}$$

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x^m}(v_m \rho\epsilon + q_m) = t_{kl}\frac{\partial v_l}{\partial x^k} + \mu_{mki}\frac{\partial \nu_{ik}}{\partial x^m} + \nu_{ik}(s_{ki} - t_{ki}) + h \tag{1.5}$$

In these equations we used the following notation: $\underline{\nu}$ is the generalized angular velocity or gyration tensor, $\underline{t}$ is the stress tensor, $\mathbf{f}$ are body forces due to external fields, $\underline{\mu}$ is the generalized coupled stress, $\underline{s} = \underline{s}^T$ is the microstress average, $\underline{l}$ are body couples due to external fields, $\mathbf{q}$ is the heat flux, and h is the heat supply due to external fields.[2] It is the purpose of this paper to give an interpretation of all these quantities in terms of microscopical variables. Moreover we want to derive Eqs. (1.1)–(1.5) from a kinetic model of a micromorphic material and to find representations for the fluxes $\underline{t}$, $\underline{\mu}$, and $\mathbf{q}$ and for the microstress average $\underline{s}$.

2. THE MODEL

In what follows we will use the kinetic model introduced in Ref. 2. We consider a system of n molecules, each composed of ν particles with the masses m^α. The state of molecule k is given by the positions $\hat{\mathbf{R}}^{k\alpha}$ and the velocities $\hat{\mathbf{V}}^{k\alpha}$ of the subparticles $\alpha = 1, \ldots, \nu$. Equivalently we may choose the center of mass $\mathbf{R}^k$, its velocity $\mathbf{V}^k$, and $2(\nu - 1)$ internal coordinates, e.g.,

$$\begin{aligned} \mathbf{R}^{k\alpha} &:= \hat{\mathbf{R}}^{k\alpha} - \hat{\mathbf{R}}^{k1} \\ \mathbf{V}^{k\alpha} &:= \hat{\mathbf{V}}^{k\alpha} - \hat{\mathbf{V}}^{k1} \end{aligned} \qquad (\alpha = 2, 3, \ldots, \nu) \tag{2.1}$$

Then, using the denotations $\mathbf{R}^{k1} := \mathbf{R}^k$ and $\mathbf{V}^{k1} := \mathbf{V}^k$ a molecule is described by the set of variables

$$X^k := (\mathbf{R}^{k1}, \ldots, \mathbf{R}^{k\nu}, \mathbf{V}^{k1}, \ldots, \mathbf{V}^{k\nu})$$

Moreover we introduce the distances and the relative velocities between particles and center of mass, i.e.,

$$\begin{aligned} \Delta\mathbf{r}^{k\alpha} &= \hat{\mathbf{R}}^{k\alpha} - \mathbf{R}^k \\ \Delta\mathbf{v}^{k\alpha} &= \hat{\mathbf{V}}^{k\alpha} - \mathbf{V}^k \end{aligned} \tag{2.2}$$

[2] $\underline{\mu}$ corresponds to the momentum $-t^{kml}$ of the microstress in Ref. 1; the symmetric $\underline{s}$ corresponds to the microstress average $\underline{t}$ introduced in Ref. 1; in (1.5) the intrinsic surface energy is omitted.

The total mass of a molecule is denoted by m. We assume three kinds of forces to act on a particle:

1. $\overset{k\alpha}{\mathbf{f}}{}^{l\beta}$: mutual force between the particles α and β of two different molecules k and l.
2. $\tilde{\mathbf{f}}^{k^{\alpha}_{\beta}}$: mutual force between the particles α and β of the same molecule k.
3. $\bar{\mathbf{f}}^{k\alpha}$: force on particle (k, α) due to external fields.

The forces $\overset{k\alpha}{\mathbf{f}}{}^{l\beta}$ and $\tilde{\mathbf{f}}^{k^{\alpha}_{\beta}}$ are assumed to have potentials $\overset{k\alpha}{u}{}^{l\beta}$ and $\tilde{u}^{k^{\alpha}_{\beta}}$. We denote the total force acting on particle (k, α) by

$$\mathbf{F}^{k\alpha} = \sum_{l=1}^{n} \sum_{\alpha_1 \beta=1}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} + \sum_{\beta=1}^{\nu} \tilde{\mathbf{f}}^{k^{\alpha}_{\beta}} + \bar{\mathbf{f}}^{k\alpha} \tag{2.3}$$

We define the potential energy of a particle by ascribing half of the energy of a pair to each of the interacting partners by

$$U^{k\alpha} = \frac{1}{2}\left(\sum_{l=1}^{n} \sum_{\beta=1}^{\nu} \overset{k\alpha}{u}{}^{l\beta} + \sum_{\beta=1}^{\nu} \tilde{u}^{k^{\alpha}_{\beta}} \right) \tag{2.4}$$

For the n-molecule distribution function of our system

$$F^{(n)}(X^1, \ldots, X^n; t)$$

Liouville's equation holds:

$$\left[\frac{\partial}{\partial t} + \sum_{k=1}^{n} \sum_{\alpha=1}^{\nu} \left(\hat{\mathbf{V}}^{k\alpha} \cdot \nabla_{\hat{\mathbf{R}}^{k\alpha}} + \frac{1}{m^{\alpha}} \mathbf{F}^{k\alpha} \cdot \nabla_{\hat{\mathbf{V}}^{k\alpha}} \right) \right] F^{(n)} = 0 \tag{2.5}$$

In this equation the arguments X^k of $F^{(n)}$ are regarded as functions of the variables $\hat{\mathbf{R}}^{k\alpha}$ and $\hat{\mathbf{V}}^{k\alpha}$.

Thus far the distribution function $F^{(n)}$ is restricted only by the condition of nonnegativity and integrability. It describes an ensemble of systems rather than a single system. In order to utilize the formalism for a derivation of the balance equations of continuum mechanics one has to impose further conditions on $F^{(n)}$. Therefore in what follows we assume that $F^{(n)}$ is macroscopically dispersionless. This implies that the mean value of a macroscopical observable A, i.e.,

$$\langle A \rangle = \int A F^{(n)}\, dX^1 \ldots dX^n \tag{2.6}$$

is identical with the value of A measured at any single system of the ensemble described by $F^{(n)}$. Hence for appropriately chosen observables A we may identify $\langle A \rangle$ with the quantities entering the balance equations of continuum physics. The balance equations themselves are given by the equations of motion for the mean values $\langle A\rangle$, i.e.,

$$\frac{\partial}{\partial t}\langle A\rangle=\left\langle \sum_{k=1}^{n}\sum_{\alpha=1}^{\nu}\left(\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}}+\frac{1}{m^{\alpha}}\mathbf{F}^{k\alpha}\cdot\nabla_{\hat{\mathbf{V}}^{k\alpha}}\right)A\right\rangle \tag{2.7}$$

which are derived easily from Liouville's equations.

3. THE MACROSCOPICAL FIELDS

In this section we introduce in our model those quantities which correspond to the fields of the phenomenological theory briefly discussed in Section 1. To this end we use as a guide the fact that the microcontinua introduced by Eringen *et al.*[1] correspond to the molecules of our model.

As usual we define the density of mass and the linear momentum by

$$\rho=\left\langle \sum_{k=1}^{n} m\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{3.1}$$

and

$$\rho\mathbf{v}=\left\langle \sum_{k=1}^{n} m\mathbf{V}^{k}\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{3.2}$$

respectively. The microinertia $\rho\underline{i}$ is given by

$$\rho\underline{i}=\left\langle \sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{r}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{3.3}$$

The generalized spin $\rho\underline{\sigma}$ is defined by

$$\rho\underline{\sigma}=\left\langle \sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{v}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{3.4}$$

so that its antisymmetric part gives the internal angular momentum of the material, while its symmetric part gives information about the deformation of the molecules.

In what follows we assume that the intramolecular forces are such that the molecules do not degenerate to dumbbells. Consequently the matrix of the components of the tensor $\underline{i}$ is nonsingular. Hence we may introduce the so-called gyration tensor $\underline{\nu}$ by

$$\underline{\sigma}^{T}=\underline{\nu}\cdot\underline{i} \tag{3.5}$$

On a microscopic level the gyration tensor $\underline{\nu}$ can be introduced as follows. Instead of using the velocities $\hat{\mathbf{V}}^{k\alpha}$ of all subparticles of a molecule we may use "collective" variables $\underline{\nu}^{k}$, $\underline{\hat{\nu}}^{k}$, etc. such that

$$\hat{\mathbf{V}}^{k\alpha}=\mathbf{V}^{k}+\underline{\nu}^{k}\cdot\Delta\mathbf{r}^{k\alpha}+\underline{\hat{\nu}}^{k}:\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{r}^{k\alpha}\cdots \tag{3.6}$$

holds. If the molecule is a rigid body, the right-hand side will stop after the second term and $\underline{\nu}^k$ will be the antisymmetric angular velocity of the molecule. But in general $\underline{\nu}^k$ is not antisymmetric for a deformable molecule, and terms of higher order are needed. In this paper we want to consider materials for which the tensor $\underline{\nu}^k$ is the only collective variable, i.e., for which the relation

$$\Delta \mathbf{v}^{k\alpha} = \bar{\underline{\nu}}^k \cdot \Delta \mathbf{r}^{k\alpha} \tag{3.7}$$

holds. Such materials are called micromorphic of degree 1. If $\bar{\underline{\nu}}^k$ is antisymmetric, i.e., if it describes a rigid rotation, the material is called polar. To simplify further calculations we introduce the additional assumption that there is no chaos among the molecules concerning their rotation and deformation, i.e., that the generalized angular velocities $\bar{\underline{\nu}}^k$ of the molecules form a macroscopically smooth field $\underline{\nu}(\mathbf{x}; t)$:[3]

$$\bar{\underline{\nu}}^k = \underline{\nu}(\mathbf{R}^k; t) \tag{3.8}$$

This assumption can be incorporated into the theory by using the distribution function $F^{(n)}$ of the special form

$$F^{(n)}(X^1, \ldots, X^n; t) = \tilde{F}^{(n)} \cdot \prod_{\substack{k=1 \ldots n \\ \alpha=1 \ldots \nu}} \delta\big(\Delta \mathbf{v}^{k\alpha} - \underline{\nu}(\mathbf{R}^k) \cdot \Delta \mathbf{r}^{k\alpha}\big) \tag{3.9}$$

where $\tilde{F}^{(n)}$ is a function of the positions of the particles and of the velocities of the centers of mass. Thus the tensor field $\underline{\nu}$ is used to describe the internal state of the medium. The assumption is physically motivated, i.e., when considering liquid crystals where macroscopic areas with well oriented molecules exist. The most general equations of balance for micromorphic materials of degree 1 are stated without proof in Appendix B.

We now define the internal energy $\rho\epsilon$ by

$$\rho\epsilon = \left\langle \sum_{k=1}^{n} \left[\frac{1}{2} m(\mathbf{V}^k - \mathbf{v})^2 + \sum_{\alpha=1}^{\nu} U^{k\alpha} \right] \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{3.10}$$

This quantity is invariant under Euclidean transformation

$$\mathbf{x}^* = \underline{Q}(t) \cdot [\mathbf{x} - \mathbf{x}_0(t)], \qquad \underline{Q}^{-1} = \underline{Q}^T \tag{3.11}$$

of the frame and the following equation holds:

$$\begin{aligned} &\rho\epsilon + \tfrac{1}{2}\rho \mathbf{v} \cdot \mathbf{v} + \tfrac{1}{2}\underline{\nu} : (\rho \underline{i} \cdot \underline{\nu}^T) \\ &= \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} \frac{1}{2} m^\alpha \hat{\mathbf{V}}^{k\alpha} \cdot \hat{\mathbf{V}}^{k\alpha} + U^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \end{aligned} \tag{3.12}$$

[3] This does not essentially restrict the theory; we only avoid the appearance of certain flux terms in the balance laws of Section 4. Moreover, this assumption is physically motivated, e.g., when considering liquid crystals, where macroscopical areas with well-oriented molecules exist.

Hence we obtain the total energy by adding the internal energy $\rho\epsilon$, the kinetic energy $\frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}$ of the macroscopical motion, and the rotational part $\frac{1}{2}\underline{\nu}:(\rho\underline{i}\cdot\underline{\nu}^T)$ of the energy. Thus definition (3.10) is motivated.

4. THE BALANCE LAWS

After having defined the macroscopical fields ρ, $\mathbf{v}$, $\underline{i}$, $\underline{\sigma}$, and ϵ, we will use Eq. (2.7) to derive the balance laws for those quantities given by (1.1)–(1.5).

4.1. Balance of Mass

With

$$A = \sum_{l=1}^{n} m\delta(\mathbf{R}^l - \mathbf{x})$$

(2.7) yields

$$\begin{aligned}\frac{\partial}{\partial t}\rho &= \left\langle \sum_{k=1}^{n}\sum_{\alpha=1}^{\nu} m\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}}\left[\sum_{l=1}^{n} m\delta(\mathbf{R}^l - \mathbf{x})\right]\right\rangle \\ &= \left\langle \sum_{k=1}^{n} m\mathbf{V}^k\cdot\nabla_{\mathbf{R}^k}\delta(\mathbf{R}^k - \mathbf{x})\right\rangle \\ &= -\nabla_{\mathbf{x}}\cdot\left\langle \sum_{k=1}^{n} m\mathbf{V}^k\delta(\mathbf{R}^k - \mathbf{x})\right\rangle \end{aligned} \tag{4.1}$$

So the well-known equation of continuity

$$\frac{\partial}{\partial t}\rho + \nabla_{\mathbf{x}}\cdot(\rho\mathbf{v}) = 0 \tag{4.2}$$

holds.

4.2. Balance of Microinertia

With

$$\begin{aligned} A &= \sum_{l=1}^{n}\left(\sum_{\beta=1}^{\nu} m^\beta\Delta\mathbf{r}^{l\beta}\otimes\Delta\mathbf{r}^{l\beta}\right)\delta(\mathbf{R}^l - \mathbf{x}) \\ &= \sum_{l=1}^{n}\left[\sum_{\beta=1}^{\nu}(m^\beta\hat{\mathbf{R}}^{l\beta}\otimes\hat{\mathbf{R}}^{l\beta}) - m\mathbf{R}^l\otimes\mathbf{R}^l\right]\delta(\mathbf{R}^l - \mathbf{x}) \end{aligned}$$

and (2.7) we obtain

$$\frac{\partial}{\partial t}(\rho\underline{i}) = \left\langle \sum_{k=1}^{n}\sum_{\alpha=1}^{\nu}(\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}})\left[\sum_{l=1}^{n}\left(\sum_{\beta=1}^{\nu} m^\beta\hat{\mathbf{R}}^{l\beta}\otimes\hat{\mathbf{R}}^{l\beta} - m\mathbf{R}^l\otimes\mathbf{R}^l\right)\times\delta(\mathbf{R}^l - \mathbf{x})\right]\right\rangle \tag{4.3}$$

Since

$$\sum_{\alpha=1}^{\nu} \hat{\mathbf{V}}^{k\alpha} \cdot \nabla_{\hat{\mathbf{R}}^{k\alpha}} \equiv \sum_{\alpha=1}^{\nu} \mathbf{V}^{k\alpha} \cdot \nabla_{\mathbf{R}^{k\alpha}} \tag{4.4}$$

holds, where $\mathbf{R}^{k\alpha}$ and $\mathbf{V}^{k\alpha}$ are the variables defined by (2.1), we get

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \underline{i}) = & -\nabla_{\mathbf{x}} \cdot \left[\left\langle \sum_{k=1}^{n} \mathbf{V}^k \otimes \left(\sum_{\alpha=1}^{\nu} m^\alpha \Delta\mathbf{r}^{k\alpha} \otimes \Delta\mathbf{r}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \right] \\ & + \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} m^\alpha \hat{\mathbf{R}}^{k\alpha} \otimes \hat{\mathbf{V}}^{k\alpha} - m\mathbf{R}^k \otimes \mathbf{V}^k \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\ & + \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} m^\alpha \hat{\mathbf{V}}^{k\alpha} \otimes \hat{\mathbf{R}}^{k\alpha} - m\mathbf{V}^k \otimes \mathbf{R}^k \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \end{aligned} \tag{4.5}$$

By denoting

$$\underline{\mathfrak{M}} := \left\langle \sum_{k=1}^{n} (\mathbf{V}^k - \mathbf{v}) \left(\sum_{\alpha=1}^{\nu} m^\alpha \Delta\mathbf{r}^{k\alpha} \otimes \Delta\mathbf{r}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.6}$$

we obtain

$$\begin{aligned} & \frac{\partial}{\partial t}(\rho \underline{i}) + \nabla_{\mathbf{x}} \cdot (\mathbf{v} \otimes \rho \underline{i} + \underline{\mathfrak{M}}) \\ & = \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} m^\alpha \Delta\mathbf{r}^{k\alpha} \otimes \Delta\mathbf{v}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\ & \quad + \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} m^\alpha \Delta\mathbf{v}^{k\alpha} \otimes \Delta\mathbf{r}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle = \rho \underline{\sigma} + \rho \underline{\sigma}^T \end{aligned} \tag{4.7}$$

Compared to Eq. (1.2) we now have found an additional flux of micro-inertia $\underline{\mathfrak{M}}$. This kinetic flux does not appear in the theory of Eringen *et al.*,[1] because that theory implies that the velocities of the microcontinua give a smooth macroscopical field. If we presume a well-ordered motion of the molecules according to

$$\mathbf{V}^k = \mathbf{v}(\mathbf{R}^k, t) \tag{4.8}$$

we will find

$$\underline{\mathfrak{M}} \equiv 0 \tag{4.9}$$

4.3. Balance of Momentum

With

$$A = \sum_{l=1}^{n} m\mathbf{V}^l \delta(\mathbf{R}^l - \mathbf{x})$$

and (2.7) we obtain (cf. Ref. 2)

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) = \left\langle \sum_{k=1}^{n} m\mathbf{V}^k(\mathbf{V}^k \cdot \nabla_{\mathbf{R}^k})\delta(\mathbf{R}^k - \mathbf{x}) \right\rangle + \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} \mathbf{F}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.10}$$

This can be written in the following form:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla_{\mathbf{x}} \cdot \left[\rho \mathbf{v} \otimes \mathbf{v} + \left\langle \sum_{k=1}^{n} m(\mathbf{V}^k - \mathbf{v}) \otimes (\mathbf{V}^k - \mathbf{v})\delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \right] = \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle + \left\langle \sum_{k=1}^{n} \sum_{\alpha=1}^{\nu} \bar{\mathbf{f}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.11}$$

because the intramolecular forces $\sum_{\alpha\beta} \tilde{\mathbf{f}}^{k\alpha}_{k\beta}$ vanish. The external forces are denoted by $\mathbf{f}$:

$$\mathbf{f} := \left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} \bar{\mathbf{f}}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.12}$$

The average over the intermolecular forces $\overset{k\alpha}{\mathbf{f}}{}^{l\beta}$ can be transformed into the divergence of a tensor field by resummation and use of formula (A.2) of the Appendix:

$$\begin{aligned} \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle &= \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \frac{1}{2} \left[\delta(\mathbf{R}^k - \mathbf{x}) - \delta(\mathbf{R}^l - \mathbf{x}) \right] \right\rangle \\ &= \nabla_{\mathbf{x}} \cdot \left\{ -\frac{1}{2} \int_0^1 \left\langle \sum_{k,l=1}^{n} (\mathbf{R}^k - \mathbf{R}^l) \otimes \left(\sum_{\alpha,\beta=1}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \right) \right. \right. \\ &\qquad \left. \left. \times \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l) \right] \right\rangle d\xi \right\} \end{aligned} \tag{4.13}$$

Thus using the abbreviations

$$\underline{t}^{\text{kin}} := -\left\langle \sum_{k=1}^{n} m(\mathbf{V}^k - \mathbf{v}) \otimes (\mathbf{V}^k - \mathbf{v})\delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.14}$$

$$\underline{t}^{\text{int}} := -\frac{1}{2} \int_0^1 \left\langle \sum_{k,l}^{n} (\mathbf{R}^k - \mathbf{R}^l) \otimes \left(\sum_{\alpha,\beta}^{\nu} \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \right) \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l) \right] \right\rangle d\xi \tag{4.15}$$

we get the balance of momentum

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla_{\mathbf{x}} \cdot \left(\rho \mathbf{v} \otimes \mathbf{v} - \underline{t}^{\text{kin}} - \underline{t}^{\text{int}} \right) = \mathbf{f} \tag{4.16}$$

So we have derived Eq. (1.3) and have obtained a representation of the stress tensor in terms of microscopical variables.

4.4. Balance of Generalized Spin

With

$$A = \sum_{l=1}^{n}\left(\sum_{\beta=1}^{\nu} m^{\beta}\,\Delta\mathbf{r}^{l\beta}\otimes\Delta\mathbf{v}^{l\beta}\right)\delta(\mathbf{R}^{l}-\mathbf{x})$$
$$= \sum_{l=1}^{n}\left(\sum_{\beta=1}^{\nu} m^{\beta}\hat{\mathbf{R}}^{l\beta}\otimes\hat{\mathbf{V}}^{l\beta} - m\mathbf{R}^{l}\otimes\mathbf{V}^{l}\right)\delta(\mathbf{R}^{l}-\mathbf{x}) \tag{4.17}$$

and with the relations

$$\left(\sum_{\alpha=1}^{\nu}\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}}\right)\mathbf{R}^{l} = \mathbf{V}^{k}\delta_{kl}$$
$$\left(\sum_{\alpha=1}^{\nu}\frac{1}{m^{\alpha}}\mathbf{F}^{k\alpha}\cdot\nabla_{\hat{\mathbf{V}}^{k\alpha}}\right)\mathbf{V}^{l} = \frac{1}{m}\left(\sum_{\alpha=1}^{\nu}\mathbf{F}^{k\alpha}\right)\delta_{kl} \tag{4.18}$$

we obtain from (2.7)

$$\frac{\partial}{\partial t}(\rho\underline{\sigma}) = -\nabla_{\mathbf{x}}\cdot\left\langle\sum_{k=1}^{n}\mathbf{V}^{k}\otimes\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\,\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{v}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle$$
$$+\left\langle\sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\hat{\mathbf{V}}^{k\alpha}\otimes\hat{\mathbf{V}}^{k\alpha} - m\mathbf{V}^{k}\otimes\mathbf{V}^{k}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle$$
$$+\left\langle\sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu}\hat{\mathbf{R}}^{k\alpha}\otimes\mathbf{F}^{k\alpha} - \mathbf{R}^{k}\otimes\sum_{\alpha=1}^{\nu}\mathbf{F}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{4.19}$$

Hence we find

$$\frac{\partial}{\partial t}(\rho\underline{\sigma}) + \nabla_{\mathbf{x}}\cdot\left[\mathbf{v}\otimes\rho\underline{\sigma} + \left\langle\sum_{k=1}^{n}(\mathbf{V}^{k}-\mathbf{v})\otimes\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\,\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{v}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle\right]$$
$$= \left\langle\sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\,\Delta\mathbf{v}^{k\alpha}\otimes\Delta\mathbf{v}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle$$
$$+\left\langle\sum_{k=1}^{n}\left(\sum_{\alpha=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\mathbf{F}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{4.20}$$

Let us introduce

$$\underline{\mu}^{\mathrm{kin}} = \left\langle\sum_{k=1}^{n}(\mathbf{V}^{k}-\mathbf{v})\otimes\left(\sum_{\alpha=1}^{\nu} m^{\alpha}\,\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{v}^{k\alpha}\right)\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \tag{4.21}$$

as the kinetic part of the spin flux. Assuming

$$\Delta \mathbf{v}^{k\alpha} = \underline{\nu}(\mathbf{R}^k, t) \cdot \Delta \mathbf{r}^{k\alpha} \tag{4.22}$$

we see that

$$\underline{\mu}^{\text{kin}} = \underline{\mathfrak{M}} \cdot \underline{\nu}^T \tag{4.23}$$

holds. Moreover we find

$$\left\langle \sum_{k=1}^{n} \left(\sum_{\alpha=1}^{\nu} m^{\alpha} \Delta \mathbf{v}^{k\alpha} \otimes \Delta \mathbf{v}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle = \underline{\nu} \cdot \rho \, \underline{i} \cdot \underline{\nu}^T \tag{4.24}$$

Splitting up the forces $\mathbf{F}^{k\alpha}$ we obtain from (4.20)

$$\begin{aligned} &\frac{\partial}{\partial t}(\rho \underline{\sigma}) + \nabla_{\mathbf{x}}\left(\mathbf{v} \otimes \rho \underline{\sigma} + \underline{\mu}^{\text{kin}}\right) \\ &\quad = \underline{\nu} \cdot \rho \, \underline{i} \cdot \underline{\nu}^T + \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\ &\qquad + \left\langle \sum_{k=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \tilde{\mathbf{f}}^{k\overset{\alpha}{\beta}} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\ &\qquad + \left\langle \sum_{k=1}^{n} \sum_{\alpha=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \bar{\mathbf{f}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \end{aligned} \tag{4.25}$$

The external (generalized) couples are denoted by $\underline{l}$:

$$\underline{l} := \left\langle \sum_{k=1}^{n} \sum_{\alpha=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \bar{\mathbf{f}}^{k\alpha} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{4.26}$$

Now we rewrite the momentum of the intermolecular forces:

$$\begin{aligned} &\left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\ &\quad = \frac{1}{2} \left\{ \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \left[\delta(\mathbf{R}^k - \mathbf{x}) - \delta(\mathbf{R}^l - \mathbf{x}) \right] \right\rangle \right. \\ &\qquad \left. + \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \left[\delta(\mathbf{R}^k - \mathbf{x}) + \delta(\mathbf{R}^l - \mathbf{x}) \right] \right\rangle \right\} \\ &\quad = \frac{1}{2} \left\{ \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta \mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \left[\delta(\mathbf{R}^k - \mathbf{x}) - \delta(\mathbf{R}^l - \mathbf{x}) \right] \right\rangle \right. \\ &\qquad \left. + \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} (\Delta \mathbf{r}^{k\alpha} - \Delta \mathbf{r}^{l\beta}) \otimes \overset{k\alpha}{\mathbf{f}}{}^{l\beta} \delta(\mathbf{R}^l - \mathbf{x}) \right\rangle \right\} \end{aligned} \tag{4.27}$$

With the formulas

$$\delta(\mathbf{R}^k - \mathbf{x}) - \delta(\mathbf{R}^l - \mathbf{x}) = -\nabla_{\mathbf{x}} \cdot \int_0^1 (\mathbf{R}^k - \mathbf{R}^l)\delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] d\xi$$

$$\delta(\mathbf{R}^l - \mathbf{x}) = \nabla_{\mathbf{x}} \cdot \int_0^1 \xi(\mathbf{R}^k - \mathbf{R}^l)\delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] d\xi + \int_0^1 \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] d\xi$$

which are derived in the Appendix we obtain

$$\begin{aligned}
&\left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} \Delta\mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \\
&= -\frac{1}{2} \nabla_{\mathbf{x}} \cdot \int_0^1 \left\langle \sum_{k,l=1}^{n} (\mathbf{R}^k - \mathbf{R}^l) \otimes \left\{ \sum_{\alpha,\beta=1}^{\nu} \left[\Delta\mathbf{r}^{k\alpha}(1-\xi) + \Delta\mathbf{r}^{l\beta}\xi\right] \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \right\} \right. \\
&\qquad \left. \times \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi \\
&\quad + \frac{1}{2} \int_0^1 \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} (\hat{\mathbf{R}}^{k\alpha} - \hat{\mathbf{R}}^{l\beta}) \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi \\
&\quad - \frac{1}{2} \int_0^1 \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} (\mathbf{R}^k - \mathbf{R}^l) \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi
\end{aligned} \tag{4.28}$$

The first term on the right-hand side of this equation is a generalized spin flux due to the intermolecular forces:

$$\begin{aligned}
\underline{\mu}^{\text{int}} &:= \frac{1}{2} \int_0^1 \left\langle \sum_{k,l=1}^{n} (\mathbf{R}^k - \mathbf{R}^l) \otimes \left[\sum_{\alpha,\beta=1}^{\nu} \left[\Delta\mathbf{r}^{k\alpha}(1-\xi) + \Delta\mathbf{r}^{l\beta}\xi\right] \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \right] \right. \\
&\qquad \left. \times \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi \\
&= \int_0^1 \left\langle \sum_{k,l=1}^{n} (\mathbf{R}^k - \mathbf{R}^l) \otimes \left(\sum_{\alpha,\beta=1}^{\nu} \Delta\mathbf{r}^{k\alpha} \otimes \overset{k\alpha}{\mathbf{f}^{l\beta}} \right)(1-\xi) \right. \\
&\qquad \left. \times \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi
\end{aligned} \tag{4.29}$$

The last identity can be derived by using the integral transformation $\xi \to 1 - \xi$ together with the exchange of the summation indices $(k, \alpha) \leftrightarrow$

(l, β) and taking into account

$$\overset{k\alpha}{\mathbf{f}}{}^{l\beta} = -\overset{l\beta}{\mathbf{f}}{}^{k\alpha} \tag{4.30}$$

This representation of the spin flux is a generalized form of formula (2.23) in Ref. 2, where the antisymmetric part of (4.29) gives the flux of the proper spin. The last term on the right-hand side of (4.28) is the interaction part $\underline{t}^{\text{int}}$ of the stress tensor. Collecting all terms we find the following balance of generalized spin:

$$\begin{aligned}\frac{\partial}{\partial t}(\rho\underline{\sigma}) &+ \nabla_{\mathbf{x}}\cdot\left(\mathbf{v}\otimes\rho\underline{\sigma} + \underline{\mu}^{\text{kin}} + \underline{\mu}^{\text{int}}\right)\\ &= \underline{\nu}\cdot\rho\underline{i}\cdot\nu^T + \underline{t}^{\text{int}} + \underline{1}\\ &\quad + \frac{1}{2}\int_0^1\left\langle\sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\hat{\mathbf{R}}^{k\alpha}-\hat{\mathbf{R}}^{l\beta})\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta\left[\mathbf{R}^k-\mathbf{x}-\xi(\mathbf{R}^k-\mathbf{R}^l)\right]\right\rangle d\xi\\ &\quad + \left\langle\sum_{k=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\Delta\mathbf{r}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k\alpha}_{k\beta})\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\end{aligned} \tag{4.31}$$

The last two terms are represented by introducing the tensor $\underline{s}$:

$$\begin{aligned}\underline{s} := &-\frac{1}{2}\int_0^1\left\langle\sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\hat{\mathbf{R}}^{k\alpha}-\hat{\mathbf{R}}^{l\beta})\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta\left[\mathbf{R}^k-\mathbf{x}-\xi(\mathbf{R}^k-\mathbf{R}^l)\right]\right\rangle d\xi\\ &-\left\langle\sum_{k=1}^{n}\left(\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k\alpha}_{k\beta}\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\end{aligned} \tag{4.32}$$

$\underline{s}$ is a symmetric tensor, because the antisymmetric parts of

$$\sum_{\alpha,\beta=1}^{\nu}(\hat{\mathbf{R}}^{k\alpha}-\hat{\mathbf{R}}^{l\beta})\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta} = \sum_{\alpha,\beta=1}^{\nu}\hat{\mathbf{R}}^{k\alpha}\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta} + \sum_{\alpha,\beta=1}^{\nu}\hat{\mathbf{R}}^{l\beta}\otimes\overset{l\beta}{\mathbf{f}}{}^{k\alpha}$$

and

$$\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k\alpha}_{k\beta} = \sum_{\alpha,\beta=1}^{\nu}\hat{\mathbf{R}}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k\alpha}_{k\beta}$$

give the vanishing total momenta of forces between two molecules and within a molecule, respectively. So we find

$$\begin{aligned}\frac{\partial}{\partial t}(\rho\underline{\sigma}) &+ \nabla_{\mathbf{x}}\cdot\left(\mathbf{v}\otimes\rho\underline{\sigma} + \underline{\mu}^{\text{kin}} + \underline{\mu}^{\text{int}}\right)\\ &= \underline{\nu}\cdot\rho\underline{i}\cdot\underline{\nu}^T + \underline{t}^{\text{int}} - \underline{s} + \underline{1}\end{aligned} \tag{4.33}$$

This verifies (1.4) if we take into account that with assumption (4.8) (which is implied in Ref. 1) the kinetic stress $\underline{t}^{\text{kin}}$ vanishes so that $\underline{t}^{\text{int}}$ is the total stress tensor.

4.5. Balance of Energy

With

$$A = \sum_{l=1}^{n}\left[\frac{1}{2}m(\mathbf{V}^l - \mathbf{v})^2 + \sum_{\beta=1}^{\nu} U^{l\beta}\right]\delta(\mathbf{R}^l - \mathbf{x})$$
$$= \sum_{l=1}^{n}\frac{1}{2}m(\mathbf{V}^l - \mathbf{v})^2\delta(\mathbf{R}^l - \mathbf{x}) + \sum_{l,m=1}^{n}\sum_{\beta,\gamma=1}^{\nu}\frac{1}{2}u^{l\beta}_{m\gamma}\delta(\mathbf{R}^l - \mathbf{x})$$
$$+ \sum_{l=1}^{n}\sum_{\beta,\gamma=1}^{\nu}\frac{1}{2}\tilde{u}^{l\beta}_{l\gamma}\delta(\mathbf{R}^l - \mathbf{x}) \tag{4.34}$$

and (2.7) we obtain

$$\frac{\partial}{\partial t}(\rho\epsilon) = \left\langle \sum_{k=1}^{n}\sum_{l=1}^{n}\left[\frac{1}{2}m(\mathbf{V}^l - \mathbf{v})^2 + \sum_{\beta=1}^{\nu} U^{l\beta}\right]\left(\sum_{\alpha=1}^{\nu}\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}}\delta(\mathbf{R}^l - \mathbf{x})\right)\right\rangle$$
$$+ \left\langle \sum_{k=1}^{n}\left[\left(\sum_{\alpha=1}^{\nu}\hat{\mathbf{V}}^{k\alpha}\cdot\nabla_{\hat{\mathbf{R}}^{k\alpha}}\right)\left(\sum_{l,m=1}^{n}\sum_{\beta,\gamma=1}^{\nu}\frac{1}{2}u^{l\beta}_{m\gamma}\right.\right.\right.$$
$$\left.\left.\left. + \sum_{l=1}^{n}\sum_{\beta,\gamma=1}^{\nu}\frac{1}{2}\tilde{u}^{l\beta}_{l\gamma}\right)\right]\delta(\mathbf{R}^l - \mathbf{x})\right\rangle$$
$$+ \left\langle \sum_{k=1}^{n}\sum_{\alpha=1}^{\nu}\frac{1}{m^{\alpha}}\mathbf{F}^{k\alpha}\cdot\nabla_{\hat{\mathbf{V}}^{k\alpha}}\left[\sum_{l=1}^{n}\frac{1}{2}m(\mathbf{V}^l - \mathbf{v})^2\right]\delta(\mathbf{R}^l - \mathbf{x})\right\rangle$$
$$=: A + B + C \tag{4.35}$$

The first term on the right-hand side can be written as

$$A = \left\langle \sum_{k=1}^{n}\left[\frac{1}{2}m(\mathbf{V}^k - \mathbf{v})^2 + \sum_{\alpha=1}^{\nu} U^{k\alpha}\right]\left[-\mathbf{V}^k\cdot\nabla_{\mathbf{x}}\delta(\mathbf{R}^k - \mathbf{x})\right]\right\rangle$$
$$= -\nabla_{\mathbf{x}}\cdot\left\{\left\langle \sum_{k=1}^{n}\mathbf{V}^k\left[\frac{1}{2}m(\mathbf{V}^k - \mathbf{v})^2 + \sum_{\alpha=1}^{\nu} U^{k\alpha}\right]\delta(\mathbf{R}^k - \mathbf{x})\right\rangle\right\}$$
$$+ \left\langle \sum_{k=1}^{n}\mathbf{V}^k\cdot\nabla_{\mathbf{x}}\left[\frac{1}{2}m(\mathbf{V}^k - \mathbf{v})^2\right]\delta(\mathbf{R}^k - \mathbf{x})\right\rangle$$
$$= -\nabla_{\mathbf{x}}\cdot(\mathbf{v}\rho\epsilon + \mathbf{q}^{\text{kin}}) + \underline{t}^{\text{kin}} : (\nabla\otimes\mathbf{v}) \tag{4.36}$$

In this equation the kinetic heat flux $\mathbf{q}^{\text{kin}}$ is defined by

$$\mathbf{q}^{\text{kin}} := \left\langle \sum_{k=1}^{n}(\mathbf{V}^k - \mathbf{v})\left[\frac{1}{2}m(\mathbf{V}^k - \mathbf{v})^2 + \sum_{\alpha=1}^{\nu} U^{k\alpha}\right]\delta(\mathbf{R}^k - \mathbf{x})\right\rangle \tag{4.37}$$

Taking into account the relations

$$\begin{aligned}\nabla_{\hat{\mathbf{R}}^{k\alpha}} u^{l\beta}_{m\gamma} &= -\overset{k\alpha}{\mathbf{f}}{}^{m\gamma}\delta_{kl}\delta_{\alpha\beta} - \overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta_{km}\delta_{\alpha\gamma}\\ \nabla_{\hat{\mathbf{R}}^{k\alpha}} \tilde{u}^{l\beta}_{\gamma} &= -\tilde{\mathbf{f}}^{k^{\alpha}_{\gamma}}\delta_{kl}\delta_{\alpha\beta} - \tilde{\mathbf{f}}^{k^{\alpha}_{\beta}}\delta_{kl}\delta_{\alpha\gamma}\end{aligned} \tag{4.38}$$

we write the second term on the right-hand side of (4.35) in the following form:

$$\begin{aligned}B = &-\frac{1}{2}\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\hat{\mathbf{V}}^{k\alpha}-\hat{\mathbf{V}}^{l\beta})\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &-\frac{1}{2}\left\langle \sum_{k=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\Delta\mathbf{v}^{k\alpha}-\Delta\mathbf{v}^{k\beta})\cdot\tilde{\mathbf{f}}^{k^{\alpha}_{\beta}}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\end{aligned} \tag{4.39}$$

The last term C yields

$$\begin{aligned}C &= \left\langle \sum_{k=1}^{n}(\mathbf{V}^k-\mathbf{v})\cdot\left(\sum_{\alpha=1}^{\nu}\mathbf{F}^{k\alpha}\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &= \left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\mathbf{V}^k\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle - \mathbf{v}\cdot\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &\quad+\left\langle \sum_{k=1}^{n}(\mathbf{V}^k-\mathbf{v})\cdot\left(\sum_{\alpha=1}^{\nu}\bar{\mathbf{f}}^{k\alpha}\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\end{aligned} \tag{4.40}$$

The last term is the heat supply h due to external forces

$$h := \left\langle \sum_{k=1}^{n}(\mathbf{V}^k-\mathbf{v})\cdot\left(\sum_{\alpha=1}^{\nu}\bar{\mathbf{f}}^{k\alpha}\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle \tag{4.41}$$

The average over the intermolecular forces $\overset{k\alpha}{\mathbf{f}}{}^{l\beta}$ can be written as divergence of the stress tensor $\underline{t}^{\text{int}}$. So we get

$$C = \left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\mathbf{V}^k\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle - \mathbf{v}\cdot\left(\nabla_{\mathbf{x}}\cdot\underline{t}^{\text{int}}\right)+h \tag{4.42}$$

Adding B and C we find

$$\begin{aligned}B+C = &\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\mathbf{V}^k+\mathbf{V}^l)\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &-\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\Delta\mathbf{v}^{k\alpha}-\Delta\mathbf{v}^{l\beta})\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &-\left\langle \sum_{k=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\Delta\mathbf{v}^{k\alpha}-\Delta\mathbf{v}^{l\beta})\cdot\tilde{\mathbf{f}}^{k^{\alpha}_{\beta}}\delta(\mathbf{R}^k-\mathbf{x})\right\rangle\\ &-\mathbf{v}\cdot\left(\nabla_{\mathbf{x}}\cdot\underline{t}^{\text{int}}\right)+h\end{aligned} \tag{4.43}$$

With the assumption (3.8), i.e.,

$$\Delta\mathbf{v}^{k\alpha} = \underline{\nu}\cdot\Delta\mathbf{r}^{k\alpha}$$

$B + C$ can be written in the following form:

$$\begin{aligned} B + C = &\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\hat{\mathbf{V}}^{k\alpha}+\hat{\mathbf{V}}^{l\beta})\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \\ &-\underline{\nu}:\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \\ &-\nu:\left\langle \sum_{k=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k}{}^{\alpha}_{\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle - \mathbf{v}\cdot\left(\nabla_{\mathbf{x}}\cdot\underline{t}^{\text{int}}\right) + h \end{aligned} \tag{4.44}$$

From the balance of spin we see that

$$\begin{aligned} &\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle + \left\langle \sum_{k=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\Delta\mathbf{r}^{k\alpha}\otimes\tilde{\mathbf{f}}^{k}{}^{\alpha}_{\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \\ &\quad = -\nabla_{\mathbf{x}}\cdot\underline{\underline{\mu}}^{\text{int}} + \underline{t}^{\text{int}} - \underline{s} \end{aligned} \tag{4.45}$$

holds. Consequently we have

$$\begin{aligned} B + C = &\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\hat{\mathbf{V}}^{k\alpha}+\hat{\mathbf{V}}^{l\beta})\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \\ &+\underline{\nu}:\left(\nabla_{\mathbf{x}}\cdot\underline{\underline{\mu}}^{\text{int}}\right)+\underline{\nu}:\left(\underline{s}-\underline{t}^{\text{int}}\right) \\ &-\mathbf{v}\cdot\left(\nabla_{\mathbf{x}}\cdot\underline{t}^{\text{int}}\right) + h \end{aligned} \tag{4.46}$$

The first term on the right-hand side of (4.46) can be transformed by resummation:

$$\begin{aligned} &\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\frac{1}{2}(\hat{\mathbf{V}}^{k\alpha}+\hat{\mathbf{V}}^{l\beta})\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta(\mathbf{R}^{k}-\mathbf{x})\right\rangle \\ &\quad = \left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}\hat{\mathbf{V}}^{k\alpha}\cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\frac{1}{2}\left[\delta(\mathbf{R}^{k}-\mathbf{x})-\delta(\mathbf{R}^{l}-\mathbf{x})\right]\right\rangle \\ &\quad = -\nabla_{\mathbf{x}}\cdot\frac{1}{2}\int_{0}^{1}\left\langle \sum_{k,l=1}^{n}\sum_{\alpha,\beta=1}^{\nu}(\mathbf{R}^{k}-\mathbf{R}^{l})(\mathbf{V}^{k}+\Delta\mathbf{v}^{k\alpha}) \right. \\ &\qquad\qquad \left. \cdot\overset{k\alpha}{\mathbf{f}}{}^{l\beta}\,\delta\!\left[\mathbf{R}^{k}-\mathbf{x}-\xi(\mathbf{R}^{k}-\mathbf{R}^{l})\right]\right\rangle d\xi \end{aligned} \tag{4.47}$$

Collecting all terms we obtain the balance of energy (written in components in a Cartesian frame):

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x^i}\left(v_i\rho\epsilon + q_i^{\text{kin}} + t_{ij}^{\text{int}} v_j - \mu_{ijk}^{\text{int}} \nu_{kj}\right)$$

$$+ \frac{\partial}{\partial x^i}\left(\frac{1}{2}\int_0^1 \left\langle \sum_{k,l=1}^{n} \sum_{\alpha,\beta=1}^{\nu} (\mathbf{R}^k - \mathbf{R}^l)_i \hat{V}_j^{k\alpha} f_j^{\substack{k\alpha \\ l\beta}}\right.\right.$$

$$\left.\left. \times\, \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi\right)$$

$$= \left(t_{ij}^{\text{kin}} + t_{ij}^{\text{int}}\right)\frac{\partial v_j}{\partial x^i} - \mu_{ijk}^{\text{int}}\frac{\partial \nu_{kj}}{\partial x^i} + \nu_{ij}\left(s_{ji} - t_{ji}^{\text{int}}\right) + h \tag{4.48}$$

Adding the last three terms on the left-hand side of this equation we define the interaction part of the heat flux by

$$\mathbf{q}^{\text{int}} = \frac{1}{2}\int_0^1 \left\langle \sum_{k,l=1}^{n} (\mathbf{R}^k - \mathbf{R}^l) \sum_{\alpha,\beta=1}^{\nu} \left[\mathbf{V}^k - \mathbf{v} + \Delta\mathbf{v}^{k\alpha}(2\xi - 1)\right] \cdot \mathbf{f}^{\substack{k\alpha \\ l\beta}}\right.$$

$$\left. \cdots\, \delta\left[\mathbf{R}^k - \mathbf{x} - \xi(\mathbf{R}^k - \mathbf{R}^l)\right] \right\rangle d\xi \tag{4.49}$$

Thus we obtain

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x^i}\left(v_i\rho\epsilon + q_i^{\text{kin}} + q_i^{\text{int}}\right)$$

$$= \left(t_{ij}^{\text{kin}} + t_{ij}^{\text{int}}\right)\frac{\partial v_j}{\partial x^i} - \mu_{ijk}^{\text{int}}\frac{\partial \nu_{kj}}{\partial x^i} + \nu_{ij}\left(s_{ji} - t_{ji}^{\text{int}}\right) + h \tag{4.50}$$

This is Eq. (1.5) if one takes into account that in Ref. 1 no kinetic fluxes appear because (4.8) is implied there.

5. SUMMARY

With the help of a kinetic model of a micromorphic material the balance laws of such a medium have been derived. The well-known equations (1.1)–(1.5) are verified for a medium of degree 1, taking into account kinetic fluxes which have been neglected in former papers about micromorphic media (see Ref. 1). Representations of stress, couple stress, and heat flux—already given in former papers[3–5]—are generalized for the micromorphic case; a representation of the symmetrical tensor $\underset{\sim}{s}$ has been found.

In the same way as is done in this paper a kinetic theory of materials of higher degree could be made; the restriction (3.8) can be dropped.

APPENDIX A

Obviously the following equations hold:

$$-\nabla_{\mathbf{x}}\cdot\int_0^1 \mathbf{y}\,\delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi = -\int_0^1 \frac{d}{d\xi}\delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi$$

$$= \delta(\mathbf{z}-\mathbf{x}) - \delta(\mathbf{z}-\mathbf{x}-\mathbf{y})$$

$$-\nabla_{\mathbf{x}}\cdot\int_0^1 \xi\mathbf{y}\,\delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi = -\int_0^1 \xi\frac{d}{d\xi}\delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi$$

$$= [\xi\delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})]_0^1 - \int_0^1 \delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi$$

$$= \delta(\mathbf{z}-\mathbf{x}-\mathbf{y}) - \int_0^1 \delta(\mathbf{z}-\mathbf{x}-\xi\mathbf{y})\,d\xi \qquad \text{(A.1)}$$

Putting $\mathbf{y}=\mathbf{R}^k-\mathbf{R}^l$; $\mathbf{z}=\mathbf{R}^k$ we obtain

$$\delta(\mathbf{R}^k-\mathbf{x}) - \delta(\mathbf{R}^l-\mathbf{x}) = -\nabla_{\mathbf{x}}\cdot\int_0^1 (\mathbf{R}^k-\mathbf{R}^l)\,\delta[\mathbf{R}^k-\mathbf{x}-\xi(\mathbf{R}^k-\mathbf{R}^l)]\,d\xi \qquad \text{(A.2)}$$

$$\delta(\mathbf{R}^l-\mathbf{x}) = \nabla_{\mathbf{x}}\cdot\int_0^1 \xi(\mathbf{R}^k-\mathbf{R}^l)\,\delta[\mathbf{R}^k-\mathbf{x}-\xi(\mathbf{R}^k-\mathbf{R}^l)]\,d\xi$$

$$+\int_0^1 \delta(\mathbf{R}^k-\mathbf{x}-\xi(\mathbf{R}^k-\mathbf{R}^l))\,d\xi \qquad \text{(A.3)}$$

APPENDIX B

We now want to state the balance laws for a degree 1 medium in their most general form by dropping assumption (3.8). The calculations are unpleasant but straightforward and of exactly the same type as those already given in the paper, so we only state the results.

Of course we will keep the definitions (3.3) and (3.4) of microinertia ρi and generalized spin $\rho\underline{\sigma}$, and again we will define the *macroscopical* gyration tensor $\underline{\nu}$ by Eq. (3.5). If this macroscopical $\underline{\nu}$ is not to describe the rotation of the molecules directly via (3.8), we will have to redefine the internal energy:

$$\rho\epsilon = \left\langle \sum_{k=1}^{n}\left(\tfrac{1}{2}m(V^k-v)^2 + \sum_{\alpha=1}^{\nu}\left(\tfrac{1}{2}m^\alpha\left[\left(\underline{\bar{\nu}}^k-\underline{\nu}\right)\cdot\Delta\mathbf{r}^{k\alpha}\right]^2 + U^{k\alpha}\right)\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle \qquad \text{(B.1)}$$

With this new $\rho\epsilon$ equation (3.12) holds without assuming (3.8), so the more general form (B.1) of the internal energy if motivated.

If we check the calculations for the balance laws, we see that the continuity equation, the balance of microinertia, and the balance of linear momentum remain unchanged. Even the balance of generalized spin holds without many changes, only (4.22) and (4.24) do not hold any more.

Defining $\underline{\mu}^{\text{kin}}$ by (4.21) as before, we see that the kinetic flux now splits up into two parts so that (4.23) has to be rewritten in the following form:

$$\underline{\mu}^{\text{kin}} = \underline{\mathfrak{M}}\cdot\underline{\nu}^T + \left\langle \sum_{k=1}^{n}(\mathbf{V}^k-\mathbf{v})\otimes\left(\underline{\bar{\nu}}^k-\underline{\nu}\right)\cdot\left(\sum_{\alpha=1}^{\nu} m^\alpha\Delta\mathbf{r}^{k\alpha}\otimes\Delta\mathbf{r}^{k\alpha}\right)\delta(\mathbf{R}^k-\mathbf{x})\right\rangle$$

$$= \underline{\mu}^{\text{kin }1} + \underline{\mu}^{\text{kin }2} \qquad \text{(B.2)}$$

Equation (4.24) has to be modified as well. Defining a symmetrical tensor

$$\underline{\lambda} = \left\langle \sum_{k=1}^{n} (\underline{\bar{v}}^k - \underline{v}) \cdot \left(\sum_{\alpha=1}^{\nu} m^\alpha \Delta \mathbf{r}^{k\alpha} \otimes \Delta \mathbf{r}^{k\alpha} \right) - (\underline{\bar{v}}^k - \underline{v}) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{B.3}$$

we obtain the balance of spin:

$$\frac{\delta}{\delta t}(\rho \underline{\sigma}) + \nabla_{\mathbf{x}} \cdot \left(\mathbf{v} \otimes \rho \underline{\sigma} + \underline{\mu}^{\text{kin 1}} + \underline{\mu}^{\text{kin 2}} + \underline{\mu}^{\text{int}} \right) = \underline{v} \cdot \rho \underline{\bar{i}} \cdot \underline{v}^T + \lambda + \underline{t}^{\text{int}} - \underline{s} + l \tag{B.4}$$

where $\underline{\mu}^{\text{int}}$, t^{int}, s, and l are defined as before.

Because of the appearance of an additional term in the definition of the internal energy $\rho\epsilon$, its balance law gives us more trouble. If we go through the procedure of 4.5 modifying the calculations where necessary we find

$$\frac{\delta}{\delta t}(\rho\epsilon) + \frac{\delta}{\delta x^i}\left(V_i \rho\epsilon + q_i^{\text{kin}} + q_i^{\text{int}} \right) = \left(t_{ij}^{\text{kin}} + t_{ij}^{\text{int}} \right) \frac{\delta v_j}{\delta x^i} - \left(\mu_{ijk}^{\text{kin 2}} + \mu_{ijk}^{\text{int}} \right) \frac{\delta v_{ml}}{\delta x^i}$$
$$+ v_{ij}\left(s_{ji} - t_{ji}^{\text{int}} - \lambda_{ij} \right) + h \tag{B.5}$$

Here $\mathbf{q}^{\text{int}}$, $\underline{t}^{\text{kin}}$, $\underline{t}^{\text{int}}$, $\underline{\mu}^{\text{int}}$, and $\underline{s}$ are defined as before, $\underline{\mu}^{\text{kin 2}}$ is given by (B.2) and $\underline{\lambda}$ by (B.3), whereas the kinetic flux $\mathbf{q}^{\text{kin}}$ and the heat supply h had to be redefined by

$$q^{\text{kin}} = \left\langle \sum_{k=1}^{n} (\mathbf{V}^k - \mathbf{v}) \left(\tfrac{1}{2} m (\mathbf{V}^k - \mathbf{v})^2 + \sum_{a=1}^{\nu} \left(\frac{m^\alpha}{2} \left[(\underline{\bar{v}}^k - \underline{v}) \cdot \Delta \mathbf{r}^{k\alpha} \right]^2 + U^{k\alpha} \right) \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle$$

$$h = \left\langle \sum_{k=1}^{n} \left(\mathbf{V}^k - \mathbf{v} + \sum_{\alpha=1}^{\nu} \left((\underline{\bar{v}}^k - \underline{v}) \cdot \Delta \mathbf{r}^{k\alpha} \right) \cdot \bar{\mathbf{f}}^{k\alpha} \right) \delta(\mathbf{R}^k - \mathbf{x}) \right\rangle \tag{B.6}$$

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