Connecting molecular dynamics to micromorphic theory. (II). Balance laws

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Abstract

In this paper, the time evolution laws for the averaged conserved dynamical variables are derived based on a molecular dynamic model. It is found that they follow exactly the balance laws in micromorphic continuum, derived by Eringen in a top-down approach. Since all the mechanical variables in micromorphic theory can be obtained from an atomic model through statistical ensemble averaging, and those averaged quantities satisfy the balance laws that govern the behavior of the continuum, it is thus concluded that the atomic model is consistent with the continuum model, and correspondence between these two models is analytically achieved. © 2003 Elsevier Science B.V. All rights reserved.

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1. Introduction

The entire physical science is based on two fundamental physical models: (1) discrete atomic models, (2) continuum field theories. While both models serve the same purpose to explain and predict physical phenomena, the descriptions are thoroughly different. The link between the two models is provided by Statistical Mechanics. The fundamental goal of Statistical Mechanics is to link the detailed determinism of many-body dynamics to the phenomenological averaged description of macroscopic behavior.

The use of “statistics” in the phenomena treated by statistical mechanics is originally dictated by the great complexity of the mechanics problems involved and by the absence of complete information defining the problems. In the case when we are only interested in some averaged values, those difficulties are balanced by the fact that only average

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aspects of the full solution are needed, and those averages are independent of the missing information.

Also, chaos forces us to take a “statistical” approach. In a real sense, chaos now provides not only an understanding of the fundamental origin of macroscopic irreversibility, but also a conceptually useful microscopic framework. Long-time solutions for individual chaotic systems are out of the question, inaccessible to any approach, analytical or numerical. Chaos requires ensemble averages.

Moreover, one of the ubiquitous variables in most experimental investigations is temperature, and this is inseparably linked to the “statistical” concept. Hence, it is not surprising that whenever the statistical mechanics of a system has been studied, it has given not only new insights into the working of the system but also new information not obtainable from purely phenomenological considerations.

The micromorphic theory is a powerful extension of the classical continuum mechanics, and has been recognized as a top-down-approach-based microcontinuum theory. This paper aims to formulate the balance laws for micromorphic continuum through a molecular dynamics model and statistical mechanics, and to investigate the correspondence between the atomic model and the micromorphic continuum theory. In Section 2, the fundamentals of the micromorphic theory are introduced; in Section 3, the statistical considerations, especially on the kinetic theory, are presented; the balance laws for micromorphic continuum based on the atomic model are derived in Section 4; the results are discussed in Section 5. Standard dyadic notations are adopted in this work.

2. The balance laws in micromorphic continuum theory

There are two essential parts in continuum field theories: the balance laws and the constitutive equations. The fundamental equations for classical continuum mechanics are the balance laws for mass, linear momentum, angular momentum, and energy and the principle of entropy. For micromorphic theory, a balance law for microinertia is added, the balance law for angular momentum is generalized to the balance law for moment of momentum, also called generalized spin, and the balance law of energy is upgraded. They are valid for all types of materials, all phases of material, namely, gas, liquid (including liquid crystal) and solid, and both equilibrium and nonequilibrium states.

In continuum mechanics, the balance laws can be written in the general form

$$\frac{d}{dt} \int_V a \, dv = \oint_S n \cdot b \, ds + \int_V c \, dv, \tag{2.1}$$

which means the rate of change of a density (per unit volume) function $a$ in a volume $V$ is equal to the flux $b$ coming in from the enclosing surface $S$ plus the source $c$ in the volume. Then the balance laws for mass, linear momentum, angular momentum, and energy can be derived.

The balance laws in micromorphic theory were originally obtained by Eringen and Suhubi [6] and Eringen [3,4] by means of a “microscopic space-averaging process”.

$$\frac{d}{dt} \int_V a \, dv = \oint_S n \cdot b \, ds + \int_V c \, dv, \tag{2.1}$$
Recently, Eringen [5] derived the balance laws of mass and microinertia by employing Eq. (2.1):

1. With \( a = \rho, b = c = 0 \), there results
   \[ \dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0 \quad (2.2) \]

2. With \( a = \rho i_{kl}, b = c = 0 \), one obtains
   \[ \frac{di}{dt} = i \cdot \omega^T + \omega \cdot i \quad (2.3) \]

Then the balance law of energy is derived with
\[ a = \rho e + \frac{1}{2} \rho v \cdot v + \frac{1}{2} \rho w \cdot i : \omega, b = t \cdot v + m : \omega + q, c = f \cdot v + l : \omega + h. \]
Finally, the balance laws of linear momentum and generalized spin are obtained by subjecting the energy balance law to the requirement of invariance under the Galilean group of transformations. Then one obtains
\[ \rho \dot{v} = \nabla \cdot t + f, \]
\[ \rho (\dot{\omega} + \omega \cdot \omega) \cdot i = \nabla \cdot m + (t - s)^T + l, \]
\[ \rho \dot{\omega} = t : \nabla \otimes v + (s - t) : \omega^T + m \cdot \nabla \otimes \omega + \nabla \cdot q + h, \]

where \( \rho, e, h, v, f, q, \omega, i, l, t, s \), and \( m \) are the mass density, internal energy, heat source, velocity, body force, heat flux, gyration, microinertia, body couple, Cauchy stress, microstress average, and moment stress, respectively. The above equations can be rewritten as
\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \]
\[ \frac{\partial}{\partial t}(\rho \mathbf{i}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{i}) = \rho \mathbf{f} + \rho \mathbf{\varphi}^T, \]
\[ \frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} - \mathbf{t}) = \mathbf{f}, \]
\[ \frac{\partial}{\partial t}(\rho \mathbf{\varphi}) + \nabla \cdot (\rho \mathbf{\varphi} \otimes \mathbf{v} - \mathbf{m}) = \mathbf{\omega} \cdot \mathbf{\omega}^T + \mathbf{t}^T - s + \mathbf{l}, \]
\[ \frac{\partial}{\partial t}(\rho \mathbf{e}) + \nabla \cdot (\rho \mathbf{e} - \mathbf{q}) = \mathbf{t} : \nabla \otimes \mathbf{v} + \mathbf{m} \cdot \nabla \otimes \mathbf{\omega} + \mathbf{\omega} : (s - t)^T + \mathbf{h}, \]

where \( \rho \mathbf{\varphi} = \mathbf{\omega} \cdot \mathbf{\varphi} \) (cf. Part I) is called the generalized spin.

3. Statistical mechanics considerations

3.1. Equation of motion for dynamical variables

The local density of the phase-space function \( \alpha(r, p) \) at point \( x \) is defined as
\[ A \equiv \sum_{k=1}^{n} \alpha(R^k, V^k) \delta(R^k - x) \equiv \sum_{k=1}^{n} \left( \sum_{z=1}^{v} \alpha(R^{kz}, V^{kz}) \right) \delta(R^k - x). \]
With the identity
\[ \nabla_{R^k} \cdot \delta(R^k - x) = -\nabla_x \cdot \delta(R^k - x) \] (3.2)
and if \( a(R^k, V^k) \) does not involve field quantities, the time derivative of \( A \) can then be expressed as
\[ \frac{\partial A}{\partial t} = \sum_{k=1}^{n} (V^k \cdot \nabla_{R^k} + V^k \cdot \nabla_{V^k})a(R^k, V^k)\delta(R^k - x) - \nabla_x \cdot (AV^k) \] (3.3)
or
\[ \frac{\partial A}{\partial t} \bigg|_{x} = \sum_{k=1}^{n} \sum_{a=1}^{v} (V^{kx} \cdot \nabla_{R^k} + V^{kx} \nabla_{V^k})a^2(R^{kx}, V^{kx})\delta(R^k - x) - \nabla_x \cdot (AV^k) . \] (3.4)

Substituting the microscopic expressions of the conserved instantaneous mechanical variables into the above equation, the local conservation laws in terms of instantaneous mechanical variables can be obtained.

The continuum field quantity is defined as the average of a dynamical function through the ensemble average [1,2]:
\[ A \equiv \langle A \rangle \equiv \int_{p} \int_{r} A(r, p, x) f(r, p, t) \, dr \, dp . \] (3.5)
The time derivative of \( \langle A \rangle \) then takes the form
\[ \frac{\partial \langle A \rangle}{\partial t} \bigg|_{x} = \left\langle \sum_{k=1}^{n} (V^k \cdot \nabla_{R^k} + V^k \cdot \nabla_{V^k})[a(R^k, V^k)\delta(R^k - x)] \right\rangle \\
+ \int_{r} \int_{p} A \dot{f} \, dr \, dp . \] (3.6)
Eq. (3.6) is the time evolution law for the averaged field quantity \( \langle A \rangle \), which depends on the rate of change of the distribution function. When \( A \) is a conserved property, the above equation yields a local conservation law for the continuum.

3.2. Equilibrium statistical mechanics

The logical foundation for Gibbs equilibrium statistical mechanics is the Liouville theorem, which describes the flow of the phase-space probability density function \( f(r, p, t) \) with \( \dot{f} = 0 \). Hence, equilibrium statistical mechanics yields the time evolution law in the following form:
\[ \frac{\partial \langle A \rangle}{\partial t} = \left\langle \sum_{k=1}^{n} (V^k \cdot \nabla_{R^k} + V^k \cdot \nabla_{V^k})[a(R^k, V^k)\delta(R^k - x)] \right\rangle . \] (3.7)
The bridge between an atomic model and continuum mechanics is then obtained in a single shot. However, most real macroscopic systems are nonequilibrium systems, and
for a nonequilibrium system no comprehensive logical foundation like Gibbs’ exists to describe the state for such systems. Kinetic theory aims to relate nonequilibrium constitutive relations to underlying atomistic force laws and to explain and describe the nonequilibrium dynamic state. The main analytical tool available for this work is the Boltzmann transport equation.

3.3. Boltzmann transport equation and nonequilibrium system

The goal of the Boltzmann transport equation is to calculate the evolution of the one-particle probability density function $f(r, p, t)$ by analyzing the effect of collisions statistically. The collision term has been obtained as the difference between a “gain” term and a “loss” term as

$$
\dot{f}_1 = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}} = \left( \frac{\partial f}{\partial t} \right)_{\text{gain}} - \left( \frac{\partial f}{\partial t} \right)_{\text{loss}}
$$

$$
= \int d\Omega \int dp_1 \sigma(\Omega)|p_1 - p_2|(f'_2 f'_1 - f_2 f_1), \tag{3.8}
$$

where $f_i = f(r, p_i, t)$, $f'_i = f(r, p'_i, t), (i = 1, 2)$. Multiplying the Boltzmann transport equation on both sides by the conserved property $A(r, p)$, and then integrating over $p$ and interchanging the integration variables $p_1, p_2, p'_1, p'_2$ with each other, we can obtain the following conservation theorem [9]:

$$
\int \int A(r, p) \left( \frac{\partial f}{\partial t} \right)_{\text{coll}} dp \, dr = 0. \tag{3.9}
$$

This means that, for conserved properties, the net change due to molecular collision is zero. Grad [7] has argued that the Boltzmann equation should be an exact statement in a gas of $N$-particles interacting via a potential. This implies that the net change for conserved properties due to particle interaction will be balanced. The Boltzmann equation thus provides a way to derive conservation laws. Based on the Boltzmann equation, conservation laws for hydrodynamics, fluid dynamics and continuum mechanics have been derived and checked with those of phenomenological field theories [9–13,16]. One of the consequences of the Boltzmann equation, therefore, is the local conservation law

$$
\frac{\partial \langle A \rangle}{\partial t} = \left\langle \sum_{k=1}^{n} (V^k \cdot \nabla R^k + \dot{V}^k \cdot \nabla V^k)[a(R^k, V^k)\delta(R^k - x)] \right\rangle. \tag{3.10}
$$

It has the same form as Eq. (3.7), but with a distribution function $f(r, p, t)$ of a nonequilibrium system, $\dot{f} \neq 0$.

Despite the approximate nature of the theorem’s derivation, the Boltzmann equation has provided an exact description for low-density gases. It satisfies the required property of implying the conservation equations, correctly identifies collisions as the mechanism leading to chaos and irreversible behavior in nonequilibrium gas systems,
and is able to explain irreversible behavior for isolated systems obeying reversible Newtonian mechanics.

3.4. Kinetic theory and the connection to continuum mechanics

The Boltzmann equation provides intimate information about gas flows, much more than those observable quantities that continuum theories take as a basic [15] Truesdell [16] has checked that the kinetic gas is in all respects a special kind of continuum, and all the requirements of continuum mechanics are satisfied by the solutions of the Boltzmann equation. Thus, the solutions represent the kinetic gas as a material in the sense of the thermodynamics of continua. The simplest gas phase theory then provides an exact analytical tool available to examine continuum theories from the viewpoint of molecular motions.

From the viewpoint of physics, the conservation equations express the basic conservation principles of physics: mass, momentum, and energy. Thus a necessary requirement for a kinetic equation to be a valid relation is that it implies these conservation laws [13]. Since the conservation laws of a continuum theory are independent of materials, the conservation laws that describe the gas dynamics would apply to the dynamics of fluid and solid as well. The consequence of the Boltzmann equation, \[ \int_r \int_p \dot{f}(r, p, t) \, dr \, dp = 0, \] for conserved properties, \( A \), is therefore employed in this work to verify the balance laws in micromorphic theory from the viewpoint of molecular motion.

4. Formulation of balance laws of micromorphic theory

The link between the instantaneous mechanical variables and the continuum field quantities has been established through the ensemble average. We use \( \tilde{A} = \langle A \rangle \) to distinguish from the corresponding instantaneous quantity \( A \). The time evolution laws in a molecular dynamics model for averaged conserved quantities under external fields are the balance laws of the continuum system. Among the mechanical variables, the mass density \( \langle \rho \rangle \), microinertia density \( \langle \rho i \rangle \), momentum density \( \langle \rho v \rangle \), generalized spin density \( \langle \rho \phi \rangle \), and the internal energy density \( \langle \rho e \rangle \) are conserved properties.

4.1. Conservation of mass

With \( \rho = \langle \sum_{k=1}^n m \delta(R^k - x) / \Delta V \rangle \), Eq. (3.10) immediately results in
\[
\frac{\partial \tilde{\rho}}{\partial t} = -\nabla \cdot \left( \sum_{k=1}^n m V^k \delta(R^k - x) / \Delta V \right). \tag{4.1}
\]
Recalling the expression for density of momentum (cf. Part I), we obtain the following well-known conservation law of mass or the equation of continuity:
\[
\frac{\partial \tilde{\rho}}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{v}) = 0. \tag{4.2}
\]
4.2. Conservation of microinertia

With \( \vec{p}_t = \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} (m^x \Delta r^{kx} \otimes \Delta r^{kx}) \delta(R^k - x)/\Delta V \right) \right\rangle \), and \( \sum_{x=1}^{v} m^x \Delta r^{kx} = 0 \), it follows that

\[
\frac{\partial}{\partial t} (\vec{p}_t) = \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} \left( V^{kx} \cdot \nabla R^k \right) \delta(R^k - x)/\Delta V \right) \right\rangle
\]

\[
= \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} m^x V^{kx} \otimes \Delta r^{kx} \right) \delta(R^k - x)/\Delta V \right\rangle
\]

\[
+ \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} m^x \Delta r^{kx} \otimes V^{kx} \right) \delta(R^k - x)/\Delta V \right\rangle
\]

\[
- \nabla_x \cdot \left\langle \sum_{k=1}^{n} V^{k} \otimes \sum_{x=1}^{v} m^x \Delta r^{kx} \otimes \Delta r^{kx} \delta(R^k - x)/\Delta V \right\rangle . \tag{4.3}
\]

Denoting

\[
\gamma \equiv \sum_{k=1}^{n} (V^k - \vec{v}) \otimes \sum_{x=1}^{v} m^x \Delta r^{kx} \otimes \Delta r^{kx} \delta(R^k - x)/\Delta V
\]

\[
= \sum_{k=1}^{n} (V^k - \vec{v}) \otimes \rho \vec{t}^k \delta(R^k - x) , \tag{4.4}
\]

its averaged value can be obtained as

\[
\langle \gamma \rangle \equiv \left\langle \sum_{k=1}^{n} (V^k - \vec{v}) \otimes \rho \vec{t}^k \delta(R^k - x) \right\rangle
\]

\[
= \int_p \int_r \sum_{k=1}^{n} (V^k - \vec{v}) \otimes \rho \vec{t}^k \delta(R^k - x) f(r, p, t) \, dr \, dp
\]

\[
= \left( \int_p (V^k - \vec{v}) f(x, p, t) \, dp \right) \otimes \rho \vec{t}^k |_{x=R^k}
\]

\[
= 0 , \tag{4.5}
\]

Hence,

\[
\frac{\partial}{\partial t} (\vec{p}_t) + \nabla_x \cdot \left( \vec{v} \otimes \vec{p}_t + \vec{\gamma} \right)
\]

\[
= \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} m^x \Delta v^{kx} \otimes \Delta v^{kx} \right) \delta(R^k - x)/\Delta V \right\rangle
\]
\[
+ \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} m^2 \Delta r^{kx} \otimes \Delta v^{kx} \right) \delta(R^k - x)/\Delta V \right\rangle
\]

\[= \bar{\rho} \bar{\varphi} + \bar{\rho} \varphi^T. \quad (4.6)\]

Therefore, the balance law of microinertia reads

\[\frac{\partial}{\partial t} (\bar{\rho} \bar{\nu}) + \nabla_x \cdot (\bar{\nu} \otimes \bar{\nu}) = \bar{\rho} \bar{\varphi} + \bar{\rho} \varphi^T. \quad (4.7)\]

It is seen that \(\langle \gamma \rangle = 0\), whereas \(\gamma \neq 0\). This means that the balance law of microinertia for instantaneous mechanical variables in an atomic model is different from that for averaged field quantities in a continuum system.

### 4.3. Balance of linear momentum

With \(\bar{\rho} \bar{\nu} = \left\langle \sum_{k=1}^{n} m V^k \delta(R^k - x)/\Delta V \right\rangle\), and

\[
\left\langle \sum_{k=1}^{n} V^k \otimes V^k \delta(R^k - x)/\Delta V \right\rangle
\]

\[= \left\langle \sum_{k=1}^{n} [(V^k - \bar{\nu}) \otimes (V^k - \bar{\nu}) + \bar{\nu} \otimes \bar{\nu}] \delta(R^k - x)/\Delta V \right\rangle, \quad (4.8)\]

it follows that

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{\nu}) = \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} \left( \frac{1}{m} \sum_{x=1}^{v} F^{kx} \right) \cdot \nabla V^k \left( \sum_{k=1}^{n} m V^k \right) \delta(R^k - x)/\Delta V \right\rangle
\]

\[-\nabla_x \cdot \left\langle \sum_{k=1}^{n} m V^k \otimes V^k \delta(R^k - x)/\Delta V \right\rangle
\]

\[= \left\langle \sum_{k=1}^{n} \left( \sum_{x=1}^{v} F^{kx} \right) \delta(R^k - x)/\Delta V \right\rangle
\]

\[-\nabla_x \cdot \left\langle \sum_{k=1}^{n} [m(V^k - \bar{\nu}) \otimes (V^k - \bar{\nu}) + \bar{\nu} \otimes \bar{\nu}] \delta(R^k - x)/\Delta V \right\rangle. \quad (4.9)\]

Because, within a unit cell \(k\), \(\sum_{x,\beta=1}^{v} f^{k\beta}_x = 0\), the above equation becomes

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{\nu}) + \nabla_x \cdot \left\langle \bar{\rho} \bar{\nu} \otimes \bar{\nu} + \sum_{k=1}^{n} m(V^k - \bar{\nu}) \otimes (V^k - \bar{\nu}) \delta(R^k - x)/\Delta V \right\rangle
\]

\[= \left\langle \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} f^{k\beta}_l \delta(R^k - x)/\Delta V \right\rangle + \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} f^{kx}_3 \delta(R^k - x)/\Delta V \right\rangle. \quad (4.10)\]
Using the identity [14]
\[
\delta(R^k - x) - \delta(R^l - x) = -\nabla_x \cdot \int_0^1 (R^k - R^l)\delta[R^k - x - \xi(R^k - R^l)]\,d\xi,
\] (4.11)
the first term on the right-hand side of Eq. (4.10) can be transformed into the divergence of \(\tilde{f}_{\text{pot}}\). Combining the definitions of the body force \(\tilde{f}\), the Cauchy stresses \(\tilde{f}_{\text{kin}}\) and \(\tilde{f}_{\text{pot}}\), there results the balance law of momentum
\[
\frac{\partial}{\partial t}(\tilde{S}^v_{\text{SSQG}}) + \nabla_x \cdot (\tilde{S}^v_{\text{SSQG}} \otimes \tilde{v} - \tilde{f}) = \tilde{f}.
\] (4.12)

### 4.4 Balance of generalized spin

With \(\tilde{\rho}\tilde{\phi} = \langle \sum_{k=1}^n \sum_{z=1}^v (m^z \Delta v^{kz} \otimes \Delta r^{kz})\delta(R^k - x)/\Delta V \rangle\), we have
\[
\frac{\partial}{\partial t}(\tilde{\rho}\tilde{\phi}) = \left\langle \sum_{k=1}^n \sum_{z=1}^v \left( V^{kz} \cdot \nabla R^{kz} + \frac{1}{m^z} F^{kz} \cdot \nabla V^{kz} \right) \times (m^z \Delta v^{kz} \otimes \Delta r^{kz})\delta(R^k - x)/\Delta V \right\rangle
\]
\[
-\nabla_x \cdot \left( \sum_{k=1}^n V^k \otimes \left( \sum_{z=1}^v m^z \Delta v^{kz} \otimes \Delta r^{kz} \right) \delta(R^k - x)/\Delta V \right).
\]
\[
= -\nabla_x \cdot \left( \sum_{k=1}^n \left( \sum_{z=1}^v m^z \Delta v^{kz} \otimes V^{kz} \right) \delta(R^k - x)/\Delta V \right)
\]
\[
+ \left( \sum_{k=1}^n \left( \sum_{z=1}^v F^{kz} \otimes \Delta r^{kz} \right) \delta(R^k - x)/\Delta V \right)
\]
\[
\equiv B + C + D.
\] (4.13)
According to the definitions of the kinetic part of moment stress and the generalized spin, and the vanishing \(\tilde{g}\), we have
\[
B = -\nabla_x \cdot \left[\tilde{v} \otimes \tilde{\rho}\tilde{\phi} \right]
\]
\[
+ \left( \sum_{k=1}^n (V^k - \bar{v}) \otimes (\omega^k - \bar{\omega} + \tilde{\omega}) \cdot \left( \sum_{z=1}^v m^z \Delta r^{kz} \otimes \Delta r^{kz} \right) \delta(R^k - x)/\Delta V \right)
\]
\[
= -\nabla_x \cdot (\tilde{v} \otimes \tilde{\rho}\tilde{\phi} - \tilde{m}^{\text{kin}}) .
\] (4.14)
Using the definitions of the microinertia, kinetic part of Cauchy stress, kinetic part of microstress average, and the definition of the generalized spin \( \tilde{\rho} \phi = \tilde{\omega} \cdot \tilde{\rho} \), there results

\[
C = \tilde{\omega} \cdot \tilde{\rho} \cdot \tilde{\omega}^T + \left( \sum_{k=1}^{n} \left( \omega^k - \tilde{\omega} \right) \cdot \left( \sum_{x=1}^{v} m^x \Delta r^{kx} \otimes \Delta r^{kz} \right) \right) \cdot \left( \omega^k - \tilde{\omega} \right)^T
\]

\[
\times \delta(R^k - x)/\Delta V
\]

\[
= \tilde{\omega} \cdot \tilde{\rho} \cdot \tilde{\omega}^T + \tilde{t}^{\text{kin}} - \tilde{s}^{\text{kin}}.
\]

(4.15)

Recalling Eq. (5.24) of Part I

\[
\nabla \cdot \tilde{m}^{\text{pot}} + (\tilde{t}^{\text{pot}} - \tilde{s}^{\text{pot}})^T
\]

\[
= \left( \sum_{k=1}^{n} \left( \sum_{l=1}^{v} \sum_{x,\beta=1}^{l} f_1^{kx} \otimes \Delta r^{kx} + \sum_{x,\beta=1}^{l} f_2^{kx} \otimes \Delta r^{kz} \right) \delta(R^k - x)/\Delta V \right),
\]

we have immediately

\[
D = \left( \sum_{k=1}^{n} \left( \sum_{l=1}^{v} \sum_{x,\beta=1}^{l} f_1^{kx} \otimes \Delta r^{kx} \right) \delta(R^k - x)/\Delta V \right)
\]

\[
= \left( \sum_{k=1}^{n} \left( \sum_{l=1}^{v} \sum_{x,\beta=1}^{l} f_1^{kx} \otimes \Delta r^{kx} + \sum_{x,\beta=1}^{l} f_2^{kx} \otimes \Delta r^{kz} \right.\right.

+ \left. \sum_{x=1}^{v} f_3^{kx} \otimes \Delta r^{kz} \right) \delta(R^k - x)/\Delta V \right)
\]

\[
= \nabla \cdot \tilde{m}^{\text{pot}} + (\tilde{t}^{\text{pot}} - \tilde{s}^{\text{pot}})^T + \tilde{l}.
\]

(4.16)

The balance law of generalized spin is thus obtained as

\[
\frac{\partial}{\partial t} (\tilde{\rho} \phi) + \nabla \cdot (\tilde{v} \otimes \tilde{\rho} \phi - \tilde{m}^{\text{kin}} - \tilde{m}^{\text{pot}})
\]

\[
= \tilde{\omega} \cdot \tilde{\rho} \cdot \tilde{\omega}^T + \tilde{t}^{\text{kin}} - \tilde{s}^{\text{kin}} + (\tilde{t}^{\text{pot}} - \tilde{s}^{\text{pot}})^T + \tilde{l}
\]

or

\[
\frac{\partial}{\partial t} (\tilde{\rho} \phi) + \nabla \cdot (\tilde{v} \otimes \tilde{\rho} \phi - \tilde{m}) = \tilde{\omega} \cdot \tilde{\rho} \cdot \tilde{\omega}^T + \tilde{t}^T - \tilde{s} + \tilde{l}.
\]

(4.17)

4.5. Conservation of energy

With

\[
\langle \rho \tilde{v} \rangle = \left( \sum_{k=1}^{n} \left[ \frac{1}{2} m(V^k - \tilde{v})^2 + \sum_{x=1}^{v} \frac{1}{2} m^x ((\omega^k - \tilde{\omega}) \cdot \Delta r^{kz})^2 \right.\right.

+ \left. \sum_{x=1}^{v} U^{kz} \right] \delta(R^k - x)/\Delta V \right).
\]
we have

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{v}) = \left\langle \sum_{k=1}^{n} \left[ \frac{1}{2} m (V^k - \bar{v})^2 + \sum_{x=1}^{v} \frac{1}{2} m^2 ((\omega^k - \bar{\omega}) \cdot \Delta r^{kx})^2 + \sum_{x=1}^{v} U^{kx} \right] \right. \\
\times (V^k \cdot \nabla_{R^k}) \delta(R^k - x) / \Delta V \\
+ \left\langle \sum_{k=1}^{n} (V^k \cdot \nabla_{R^k}) \left[ \frac{1}{2} m (V^k - \bar{v})^2 + \sum_{x=1}^{v} \frac{1}{2} m^2 ((\omega^k - \bar{\omega}) \cdot \Delta r^{kx})^2 \\
+ \sum_{x=1}^{v} U^{kx} \right] \delta(R^k - x) / \Delta V \right. \\
+ \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} \left( \frac{1}{m^2} F^{kx} \cdot \nabla_{V^{kx}} \right) \left[ \frac{1}{2} m (V^k - \bar{v})^2 \\
+ \sum_{x=1}^{v} \frac{1}{2} m^2 ((\omega^k - \bar{\omega}) \cdot \Delta r^{kx})^2 + \sum_{x=1}^{v} U^{kx} \right] \delta(R^k - x) / \Delta V \right. \\
\equiv P + Q + R ,
\]

where \(P, Q,\) and \(R\) can be further derived as follows:

\[
P = - \nabla_{x} \cdot \left\langle \sum_{k=1}^{n} (V^k - \bar{v} + \bar{\omega}) \left[ \frac{1}{2} m (V^k - \bar{v})^2 + \sum_{x=1}^{v} \frac{1}{2} m^2 ((\omega^k - \bar{\omega}) \cdot \Delta r^{kx})^2 \right. \\
+ \sum_{x=1}^{v} U^{kx} \right] \delta(R^k - x) / \Delta V \\
+ \left\langle \sum_{k=1}^{n} (V^k - \bar{v} + \bar{\omega}) \cdot \nabla_{x} \left( \frac{1}{2} m (V^k - \bar{v})^2 \\
+ \sum_{x=1}^{v} \frac{1}{2} m^2 ((\omega^k - \bar{\omega}) \cdot \Delta r^{kx})^2 \right) \delta(R^k - x) / \Delta V \right. \\
= - \nabla_{x} \cdot (\bar{v} \bar{\rho} \bar{v} - \bar{\rho}^{kin}) \\
- \left\langle \sum_{k=1}^{n} (V^k - \bar{v} + \bar{\omega}) \otimes \left( m(V^k - \bar{v}) : \nabla_{x} \otimes \bar{v} \\
+ \sum_{x=1}^{v} m^2 (\omega^k - \bar{\omega}) \cdot \Delta r^{kx} : \nabla_{x} \otimes (\bar{\omega} \cdot \Delta r^{kx}) \right) \delta(R^k - x) / \Delta V \right. \\
\]

\(\equiv\)
\[ P = -\nabla_x \cdot (\tilde{v} \tilde{p} \tilde{e} - \tilde{q}^{\text{kin}}) + \tilde{r}^{\text{kin}} : \nabla_x \otimes \tilde{v} + \tilde{m}^{\text{kin}} : \nabla_x \otimes \tilde{\omega} \]

\[ = -\nabla_x \cdot (\tilde{v} \tilde{p} \tilde{e} - \tilde{q}^{\text{kin}}) + \tilde{r}^{\text{kin}} : \nabla_x \otimes \tilde{v} + \tilde{m}^{\text{kin}} : \nabla_x \otimes \tilde{\omega} \]

\[ = -\left( \sum_{k=1}^{n} \tilde{v} \otimes \left( m(V^k - \tilde{v}) : \nabla_x \otimes \tilde{v} \right) \right) \]

\[ + \sum_{x=1}^{v} m^x (\omega^k - \tilde{\omega}) \cdot \Delta r^{kx} : \nabla_x \otimes (\tilde{\omega} \cdot \Delta r^{kx}) \right) \delta(R^k - x) / \Delta V \right) . \quad (4.19) \]

According to the definitions of linear momentum and generalized spin, the last term on the right-hand side of the above equation vanishes. This leaves

\[ P = -\nabla_x \cdot (\tilde{v} \tilde{p} \tilde{e} - \tilde{q}^{\text{kin}}) + \tilde{r}^{\text{kin}} : \nabla_x \otimes \tilde{v} + \tilde{m}^{\text{kin}} : \nabla_x \otimes \tilde{\omega} . \quad (4.20) \]

Taking into account the relations

\[ \nabla_{R^{kx}} u_1^{l_\beta} = -f_1^{m_\gamma} \delta_{l_\beta} \delta_{x_\gamma} , \]

\[ \nabla_{R^{kx}} u_2^{l_\beta} = -f_2^{k_\gamma} \delta_{l_\beta} \delta_{x_\gamma} - f_2^{k_\gamma} \delta_{k_\beta} \delta_{x_\gamma} , \quad (4.21) \]

and recalling the definitions of \( s^{\text{kin}} \), \( t^{\text{kin}} \), and \( \langle \rho \phi \rangle = \langle \omega \cdot \rho \tilde{t} \rangle = \langle \omega \rangle \cdot \langle \rho \tilde{t} \rangle \), \( Q \) becomes

\[ Q = \left( \sum_{k=1}^{n} \sum_{x=1}^{v} (V^{kx} : \nabla_{R^{kx}}) \left[ \sum_{l=1}^{n} \sum_{\beta=1}^{v} u_1^{l_\beta} + \sum_{\beta=1}^{v} u_2^{l_\beta} \right] \right) \]

\[ + \frac{1}{2} m^x (\Delta v^{kx} - \tilde{\omega} \cdot \Delta r^{kx})^2 \right) \delta(R^k - x) / \Delta V \right) \]

\[ = -\frac{1}{2} \left( \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^{kx} - V^{l_\beta}) \cdot f_1^{k_\gamma} \delta(R^k - x) / \Delta V \right) \]

\[ -\frac{1}{2} \left( \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^{kx} - V^{l_\beta}) \cdot f_2^{k_\gamma} \delta(R^k - x) / \Delta V \right) \]

\[ - \left( \sum_{k=1}^{n} \sum_{x=1}^{v} m^x [(\omega^k - \tilde{\omega} + \tilde{\omega}) \cdot \Delta r^{kx} \otimes (\omega^k - \tilde{\omega}) \cdot \Delta r^{kx} : \tilde{\omega}] \delta(R^k - x) / \Delta V \right) \]

\[ = -\frac{1}{2} \left( \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^{kx} - V^{l_\beta}) \cdot f_1^{k_\gamma} \delta(R^k - x) / \Delta V \right) \]

\[ - \left( \sum_{k=1}^{n} \left( \sum_{x,\beta=1}^{v} \Delta v^{kx} \cdot f_2^{k_\gamma} \right) \delta(R^k - x) / \Delta V \right) \]

\[ + \tilde{\omega} : (\tilde{s}^{\text{kin}} - \tilde{t}^{\text{kin}}) . \quad (4.22) \]
If we hold to the usual viewpoint that the potential energy $U^{kz}$ is not a function of atomic velocity $V^{kz}$, then

$$R = \left\langle \sum_{k=1}^{n} \sum_{\beta=1}^{v} \frac{1}{m^\beta} F^{k\beta} \cdot \nabla \nu^\beta \left( \frac{1}{2} m (V^k - \vec{v})^2 + \sum_{x=1}^{v} \frac{1}{2} m^x ((\omega^k - \vec{\omega}) \cdot \Delta r^{kx})^2 \right) \right\rangle \delta(R^k - x)/\Delta V$$

$$= \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} (V^k - \vec{v} + (\omega^k - \vec{\omega}) \cdot \Delta r^{kx}) \cdot F^{kx} \delta(R^k - x)/\Delta V \right\rangle$$

$$= \left\langle \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^k - \vec{v}) \cdot f_{1,1}^{k\beta} \delta(R^k - x)/\Delta V \right\rangle$$

$$+ \left\langle \sum_{k=1}^{n} \sum_{x,\beta=1}^{v} (\omega^k - \vec{\omega}) \cdot \Delta r^{kx} \cdot \left( \sum_{l=1}^{n} f_{1,1}^{k\beta} + f_{2,2}^{k\beta} \right) \delta(R^k - x)/\Delta V \right\rangle$$

$$+ \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} (V^k - \vec{v} + (\omega^k - \vec{\omega}) \cdot \Delta r^{kx}) \cdot f_{3}^{kx} \delta(R^k - x)/\Delta V \right\rangle . \quad (4.23)$$

Denoting

$$\lambda \equiv \sum_{k=1}^{n} \sum_{x=1}^{v} (V^k - \vec{v} + (\omega^k - \vec{\omega}) \cdot \Delta r^{kx}) \cdot f_{3}^{kx} \delta(R^k - x)/\Delta V , \quad (4.24)$$

it follows that

$$Q + R = -\frac{1}{2} \left\langle \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^{kz} - V^{l\beta}) \cdot f_{1,1}^{k\beta} \delta(R^k - x)/\Delta V \right\rangle$$

$$- \left\langle \sum_{k=1}^{n} \left( \sum_{x,\beta=1}^{v} \Delta v^{kz} \cdot f_{2,2}^{k\beta} \right) \delta(R^k - x)/\Delta V \right\rangle + \vec{\omega} : (\vec{s}^{kin} - \vec{r}^{kin})$$

$$+ \left\langle \sum_{k,l=1}^{n} \sum_{x,\beta=1}^{v} (V^k - \vec{v}) \cdot f_{1,1}^{l\beta} \delta(R^k - x)/\Delta V \right\rangle$$
\begin{align*}
+ \left( \sum_{k=1}^{n} \sum_{x, \beta = 1}^{v} (\omega^k - \bar{\omega}) \cdot \Delta r^k \cdot \left( \sum_{l=1}^{n} f_1^{k \beta} + f_2^{k \beta} \right) \delta(R^k - x)/\Delta V \right) + \bar{\lambda} \\
= \left( \sum_{k,l=1}^{n} \sum_{x, \beta = 1}^{v} \frac{1}{2} (V^{k \beta} + \bar{V}^{l \beta}) \cdot f_1^{k \beta} \delta(R^k - x)/\Delta V \right) - \bar{\nu} \cdot (\nabla_x \cdot \bar{\tau}^\text{pot}) \\
- \bar{\omega} : (\nabla_x \cdot \bar{\mathbf{m}}^\text{pot} + (\bar{\mathbf{t}}^\text{pot} - \bar{s}^\text{pot})^T) + \bar{\omega} : (\bar{s}^\text{kin} - \bar{\mathbf{t}}^\text{kin}) + \bar{\lambda}. \tag{4.25}
\end{align*}

With Eq. (5.25) in Part I,
\begin{align*}
\nabla_x \cdot \left( \bar{\mathbf{Q}}^\text{pot} + \bar{\mathbf{m}}^\text{pot} : \bar{\omega} + \bar{\mathbf{t}}^\text{pot} \cdot \bar{\nu} \right) \\
= \frac{1}{2} \left( \sum_{k,l=1}^{n} \sum_{x, \beta = 1}^{v} (V^{k \beta} + \bar{V}^{l \beta}) \cdot f_1^{k \beta} \delta(R^k - x)/\Delta V \right),
\end{align*}
we have
\begin{align*}
P + Q + R \\
= - \nabla_x \cdot \left( \bar{\mathbf{v}}^\text{pot} - \bar{\mathbf{q}}^\text{kin} \right) + \left( \bar{\mathbf{t}}^\text{kin} + \bar{\mathbf{p}}^\text{pot} \right) : (\nabla_x \otimes \bar{\nu}) \\
+ (\bar{\mathbf{m}}^\text{pot} + \bar{\mathbf{m}}^\text{kin}) : (\nabla \otimes \bar{\omega}) + \bar{\omega} : (\bar{s} - \bar{\mathbf{t}})^T \\
+ \bar{\lambda} + \nabla_x \cdot \left( \bar{\mathbf{Q}}^\text{pot} + \bar{\mathbf{m}}^\text{pot} : \bar{\omega} + \bar{\mathbf{t}}^\text{pot} \cdot \bar{\nu} \right) \\
- \nabla_x \cdot (\bar{\mathbf{m}}^\text{pot} : \bar{\omega}) - \nabla_x \cdot (\bar{\mathbf{t}}^\text{pot} \cdot \bar{\nu}). \tag{4.26}
\end{align*}
The balance law of energy is finally obtained as
\begin{align*}
\frac{\partial (\rho \bar{w})}{\partial t} + \nabla \cdot \left( \bar{\mathbf{v}}^\text{pot} - \bar{\mathbf{q}} \right) = \bar{\mathbf{t}} : \nabla \otimes \bar{\mathbf{v}} + \bar{\mathbf{m}} : \nabla \otimes \bar{\omega} + \bar{\omega} : (\bar{s} - \bar{\mathbf{t}})^T + \bar{\lambda}. \tag{4.27}
\end{align*}
Here the source of mechanical energy is taken into consideration. If an energy source of nonmechanical origin, denoted by \( \bar{h} \), is included, then the balance law of energy can be obtained as
\begin{align*}
\frac{\partial (\rho \bar{e})}{\partial t} + \nabla \cdot \left( \bar{\mathbf{v}}^\text{pot} - \bar{\mathbf{q}} \right) = \bar{\mathbf{t}} : \nabla \otimes \bar{\mathbf{v}} + \bar{\mathbf{m}} : \nabla \otimes \bar{\omega} + \bar{\omega} : (\bar{s} - \bar{\mathbf{t}})^T + \bar{\lambda} + \rho \bar{h}. \tag{4.28}
\end{align*}

5. Discussion

Comparing the balance laws introduced in Section 2 with those derived in Section 4, it is seen that the first four equations are identical, while the energy equation has an additional term
\begin{align*}
\bar{\lambda} \equiv \left( \sum_{k=1}^{n} \sum_{x=1}^{v} (V^k - \bar{\mathbf{v}} + (\omega^k - \bar{\omega}) \cdot \Delta r^k) \cdot f_3^{k \beta} \delta(R^k - x)/\Delta V \right), \tag{5.1}
\end{align*}
where $f^{kz}_3$ is body force on atom $(k, z)$ due to external fields. If the external field is the gravitational field, i.e., $f^{kz}_3 = m^2g$, then $I = 0$ and

$$\tilde{\lambda} = \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} (V^k - \tilde{v} + (\omega^k - \tilde{\omega}) \cdot \Delta r^{kz}) \cdot f^{kz}_3 \delta(R^k - x)/\Delta V \right\rangle$$

$$= \left\langle \sum_{k=1}^{n} \sum_{x=1}^{v} m^2(V^k - \tilde{v} + (\omega^k - \tilde{\omega}) \cdot \Delta r^{kz}) \delta(R^k - x)/\Delta V \right\rangle \cdot g = 0.$$

If the external field is not the gravitational field, e.g., electromagnetic attractions, then both $I$ and $\tilde{\lambda}$ would not vanish, and this is also concluded by Eringen [5]. Therefore, the balance laws derived in this chapter based on the Boltzmann equation agree exactly with those derived by Eringen [5] in a top-down approach.

On the other hand, it is noticed that $\gamma$ and $\lambda$ vanish, whereas $\gamma$ and $\lambda$ are non-vanishing. This implies that the balance laws for instantaneous mechanical variables and for continuum field quantities are different. Hence the continuum forms of the balance laws only hold in the statistical sense. This conclusion may be of particular importance as interests in the multi-scale modeling increase and various integrations of models and theories are proposed. This work shows that the gap between some theories or models, which are well established in their own right, cannot be bridged without a serious theoretical reconstruction.

Recall that the time-evolution law from the Liouville theorem and that from the Boltzmann equation for conserved properties take the same form. Hence equilibrium statistical mechanics and nonequilibrium statistical mechanics of gas system yield the same balance laws. The conceptual basis of macroscopic thermodynamics and microscopic statistical mechanics is the ideal gas which makes it possible to give quantitative definitions of pressure and temperature, to calculate the classical and quantum partition functions, and to link these two approaches through Bohr’s Correspondence Principle [8]. In this work, the simple ideal gas model has enabled us to derive the balance laws of Micromorphic Theory, and we have verified that the time evolution laws of averaged conserved properties in the molecular dynamics model agree exactly with the balance laws obtained by Eringen. If an exact analytical kinetic theory for solids is available, it is reasonable to believe that the form of the balance laws derived should be the same as those obtained here.

Since all the mechanical variables in the micromorphic field theory can be obtained from an atomic model through statistical ensemble averages, and those averaged quantities satisfy the same fundamental equations of balance laws that govern the behavior of the continuum, it is thus concluded that the atomic model is consistent with the continuum model, and that the correspondence between this two models can be achieved whenever an ensemble averaging is meaningful.

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References