THE MOTIVATION OF CONTINUUM CONCEPTS AND RELATIONS FROM DISCRETE CONSIDERATIONS

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SUMMARY

Fundamental concepts and balance relations employed in continuum mechanics are motivated on the basis of atomistic considerations together with a naïve treatment of thermal motion.

1. Introduction

THE macroscopic behaviour of a given material derives from its (discrete) microstructure. In modelling the material as a continuous body (cf. Truesdell and Noll (**1**)) it is desirable to be able to relate continuum parameters, balance equations, and constitutive relations to this microstructure in order both to gain insight into the physical significance of the parameters and their inter-relations, and to delimit the validity of the model employed. In order to discuss this relationship it is necessary to employ a model of the microstructure in question, the simplest of which takes the body to be an assembly of interacting particles (point masses). Adopting such a viewpoint, the basic concepts and balance relations of continuum mechanics are here motivated, a naïve approach to the fundamentally erratic behaviour of matter at the atomic level (that is, thermal motion and consequent fluctuations in physical parameters) being employed which nevertheless provides insight into the concepts of heat content, conduction, and radiation in both solid and fluid phases.

In section 2 the concepts of (mass) density and velocity are motivated for a system of particles (modelling atoms, ions, or molecules), the latter being used to formulate the notions of material point and motion and also mandating mass conservation. Balances of linear and rotational momentum and of energy are derived for solids in section 3 using the particle model, but no account is taken of thermal motion. Linear momentum balance is shown to hold as a consequence of two basic assumptions: namely, that there is no net self-force associated with all particles within any region of macroscopic proportion (for definiteness, a region having 10^{-4} m as the smallest dimension associated with any feature thereof) and that the net force exerted on an individual particle due to its interaction with all other particles derives only from those within a distance of 10^3 Å (10^{-7} m). It is the second of these

which results in the concept of traction and hence stress. The integral form of the relation for a macroscopic region R is obtained by summing the equations of motion for all particles therein and then decomposing the sum into contributions from volume cells of characteristic dimension 10^{-5} m and surface cells of characteristic dimensions $10^{-5}\,\mathrm{m}\times 10^{-5}\,\mathrm{m}\times 10^{-7}$ m. Tensorially pre-multiplying the aforementioned equations of motion by the instantaneous displacement of the particles concerned from an arbitrary fixed point and summing over R yields, in similar manner, a generalised moment of momentum balance in integral form whose skew part corresponds to rotational momentum balance. Under the additional assumptions that particles within any region of macroscopic proportion experience no net self-couple, and that, locally, particle distributions deform homogeneously (in the absence of thermal motion this is regarded to be a good approximation for solids and is the only aspect of the discussion which limits this to solid phases), the resulting relation differs from its usual form only in having a term corresponding to couple-stress (other terms are present but demonstrably negligible as a consequence of the second of these additional assumptions). This is seen to be a local measure of inhomogeneity and arguably negligible. Energy balance is obtained in like manner on summing the scalar multiples of individual equations of motion with the relevant particle velocities. For interactions governed by separation-dependent pair-potentials the internal energy is identified with binding energy, an alternative being discussed for more general situations. Remarks are made on changes of frame and invariance of the energy equation under superposed rigid motions. Section 4 takes account of thermal motion in solids and fluids, distinguishing between these, the balance laws being motivated by taking time averages of equations obtained in the manner of section 3. Included in these relations are terms identifiable with heat flux, heat content, and radiation. These quantities are defined in terms of individual particle velocity relative to the macroscopic velocity at the instantaneous location of the particle, admitting a common definition for each, irrespective of whether the phase in question is solid or fluid. Among other parameters, the traction, heat flux, heat content, and radiative heat supply are shown to take objective values provided all observers agree upon those quantities which are subject to fluctuation. Concluding remarks on generalisations and possible implications of this work are made in section 5.

The arguments presented herein which relate to spatial and temporal averaging, while physically natural and plausible, are not precise mathematical statements. However, these provide compelling reasons for making the technical assumptions upon which a rigorous mathematical treatment of material behaviour may be based, namely continuum mechanics, simultaneously delimiting the expected range of validity of this viewpoint. An alternative approach, in which the averaging procedures are rendered precise, is provided by statistical mechanics, but, in view of the limited objectives of

this study, it is not here necessary to invoke the philosophy and formalism of this discipline.

Given that many of the ideas discussed have long been appreciated (for example, correlation of the short-range nature of molecular interactions with the notion of stress, and of heat with erratic microscopic motion), some justification for this particular contribution is in order. In this respect it is felt that assumptions inherent in the adoption of a continuum model for material behaviour are rendered particularly clear by the formalism here developed which involves pseudo-limits of sums taken over so-called ε-cells. Reasons for the greater generality of the classical form of linear, as compared with rotational, momentum balance become transparent, and it is shown why the energy equation is invariant under superposed rigid motions. Thermal considerations are treated in a manner which underlines the fundamental difference between microscopic motions in fluids and in solids. The analysis of the manner in which continuum parameters transform under frame changes as a consequence of their definitions in terms of atomistic quantities is instructive in view of the current controversy concerning the principle of material frame-indifference (cf. Müller (**2**), Edelen and McLennan (**3**), Woods (**4**), Wang (**5**), and Speziale (**6**)). Further, this work readily serves as a starting point from which to discuss mixture theories (cf. Atkin and Craine (**7**)) and also to analyse the physical significance of parameters in theories of generalised continua (cf. Kröner (**8**)). In respect of the latter it is hoped in subsequent work to be able to delineate situations in which there are good *a priori* reasons for believing a particular theory to be appropriate, as distinct from *a posteriori* adjustment of material parameters to fit experimental data. Here we have in mind fluids consisting of large molecules, (in particular, liquid crystalline phases: cf. de Gennes (**9**)), granular materials, suspensions and emulsions, and emphasize that a given model might only be expected to be appropriate for certain motions or under specific conditions. Finally, doubt is cast upon the physical motivation underlying theories of non-local interactions (cf. Edelen (**10**)), since molecular physicists (cf. Hirschfelder, in (**11**)) term "very long range" those interactions which extend to 200 Å, while here it is shown how interactions of range 1000 Å result only in local continuum theories.

2. Basic considerations

A body is here regarded as a system of interacting point masses which model atoms, ions, or molecules, a typical particle P_i having mass m_i. If $S_\varepsilon(\mathbf{x})$ denotes the interior of the sphere centred at the geometrical point $\mathbf{x}$ with radius ε then

$$\rho_\varepsilon(\mathbf{x}, t) := \sum_i m_i \Big/ V_\varepsilon, \tag{2.1}$$

where the sum is taken over particles within $S_\varepsilon(\mathbf{x})$ at instant t and V_ε

denotes the volume of the sphere. Now let ε range over values macroscopically small but microscopically large, say ε of order 10^{-5} m (10^5 Å) for definiteness. (Nearest-neighbour separation in a solid (or liquid) phase is of order 1–10 Å, so that a cubic lattice structure of side 10 Å would yield 10^{15} atoms in a cube of side 10^{-5} m.) If $\rho_\varepsilon(\mathbf{x}, t)$ is constant (more precisely, constant to within a certain high degree of accuracy, since the graph of $\rho_\varepsilon(\mathbf{x}, t)$ as a function of ε will consist of very many disjoint pieces, each of which has inverse cubic form) over an interval within this range then this (assumed unique) value is denoted by $\lim_\varepsilon \{\rho_\varepsilon(\mathbf{x}, t)\}$, and termed the density ρ at $(\mathbf{x}, t)$: that is,

$$\rho(\mathbf{x}, t) := \lim_\varepsilon \{\rho_\varepsilon(\mathbf{x}, t)\}. \tag{2.2}$$

The foregoing may be modified to introduce some shape insensitivity: any simply-connected convex open set S of span 2ε which includes $S_{\varepsilon/2}(\mathbf{x})$ and is balanced about $\mathbf{x}$ (that is, $\mathbf{x}-\mathbf{u}\in S$ whenever $\mathbf{x}+\mathbf{u}\in S$) will be termed an *$\varepsilon$-cell centred at* $\mathbf{x}$. (Of course, the choice $S_{\varepsilon/2}(\mathbf{x})$ is somewhat arbitrary: it is, however, insufficient to insist only upon the span and convexity criteria since then it may be possible to choose cells which contain no particles whatsoever, for any ε.) In particular, cubical boxes centred at $\mathbf{x}$ of span 2ε and arbitrary orientation are included in this category. Definition (2.2) is now assumed to be meaningful with ρ_ε given by (2.1) in respect of ε-cells centred at $\mathbf{x}$, V_ε denoting the cell volume. The definition suggests that ρ varies spatially very little at the 10^{-5} m scale. It is also possible to argue that ρ is not subject to fluctuation. These observations motivate the basic assumption that ρ be continuous; in fact ρ is assumed to be of class C^1. Having made this technical assumption it is important to realise that while it is conventional to impose no further restrictions upon ρ, analyses which allow ρ to vary substantially on ε length- or atomistic time-scales are at variance with the continuum viewpoint as here presented.

Since surface effects are not considered here ρ is taken to be defined everywhere, the region occupied by the body at any instant t being identified with the (necessarily open) set $\{\mathbf{x}: \rho(\mathbf{x}, t) > 0\}$.

The macroscopic velocity field $\mathbf{v}$ is derived in similar fashion: if $\mathbf{v}_i$ denotes the velocity of m_i, then

$$\mathbf{v}(\mathbf{x}, t) := \lim_\varepsilon \{\mathbf{v}_\varepsilon(\mathbf{x}, t)\},$$

where

$$\mathbf{v}_\varepsilon(\mathbf{x}, t) := \sum_i m_i \mathbf{v}_i \Big/ \sum_i m_i. \tag{2.3}$$

Of course, the sums are over particles in an ε-cell centred at $\mathbf{x}$ at instant t. It is to be noted that the scale of the cells used, together with the notion of ε-limit, is consistent with the neglect of quantum mechanical considerations. As with ρ, $\mathbf{v}$ is assumed to be of class C^1.

If R denotes a region of macroscopic proportions (that is, a region which can be divided up into many ε-cells) then the mass and linear momentum to be associated therewith are, by virtue of (2.1), (2.2) and (2.3), to be identified with the Riemann integrals of respectively ρ and $\rho\mathbf{v}$ over R. That similar interpretations be made for regions of ε-cell dimension with $\varepsilon \sim 10^{-5}$ m is consistent with the (assumed) insensitivity of these parameters at this scale which ensures the existence of the ε-limits. However, although integrals over arbitrarily small regions are defined, their values clearly cannot be identified with the mass or linear momentum therein when these regions are smaller than those for which the ε-limits exist.

It is now possible to motivate the concepts of material point and motion thereof. Let $\hat{\mathbf{x}} \in B$, where B is the (open) region occupied by the body at any instant $\hat{t}$, and consider the initial-value problem of determining $\boldsymbol{\chi}(\hat{\mathbf{x}}, t)$ from

$$\dot{\boldsymbol{\chi}}(\hat{\mathbf{x}}, t) = \mathbf{v}(\boldsymbol{\chi}(\hat{\mathbf{x}}, t), t), \qquad \boldsymbol{\chi}(\hat{\mathbf{x}}, \hat{t}) = \hat{\mathbf{x}}. \tag{2.4}$$

It is assumed that a unique solution exists for all t in some open interval containing $\hat{t}$ (I say) for all $\hat{\mathbf{x}} \in B$, and with each $\hat{\mathbf{x}}$ is identified a material point (X say) whose location at instant t is defined to be $\boldsymbol{\chi}(\hat{\mathbf{x}}, t)$. The map $\boldsymbol{\chi}(\hat{\mathbf{x}}, .): I \to \mathscr{E}$ (three-dimensional Euclidean space) is termed the motion of X relative to the instantaneous configuration B. It follows that two distinct material points can never simultaneously occupy the same geometrical point, since, by uniqueness, were they to coincide at some instant ($\hat{t}$ say) they would coincide throughout the motion and hence be indistinguishable.

The notions of material and spatial time derivatives in respect of any parameter f defined on the trajectory of the body follow in standard fashion (cf. Truesdell and Toupin (**12**), §72) being denoted by $\dot{f}$ and f' respectively. In particular, the acceleration field $\mathbf{a}$ is defined as the material time derivative of the velocity field $\mathbf{v}$:

$$\mathbf{a}(\mathbf{x}, t) := \dot{\mathbf{v}}(\mathbf{x}, t) = \ddot{\boldsymbol{\chi}}(\hat{\mathbf{x}}, t),$$

where $\mathbf{x} = \boldsymbol{\chi}(\hat{\mathbf{x}}, t)$.

If R denotes any regular region (cf. Kellogg (**13**), p. 113) of macroscopic proportions then the time rate of change of mass therein will derive solely from mass influx (or efflux) across its boundary ∂R. This must be identified with the integral thereover of $-\rho\mathbf{v}.\mathbf{n}$, where $\mathbf{n}$ denotes the outward unit normal to ∂R. Thus

$$\frac{d}{dt}\int_R \rho = -\int_{\partial R} \rho\mathbf{v}.\mathbf{n}. \tag{2.5}$$

It follows that

$$0 = \int_R (\dot{\rho} + \rho \operatorname{div} \mathbf{v}) = \int_{R_0} \widehat{\rho J} = \frac{d}{dt}\int_{R_t} \rho. \tag{2.6}$$

Here J denotes the Jacobian of $\boldsymbol{\chi}(., t)$ and $R_t := \boldsymbol{\chi}(R_0, t)$, R_t instantaneously

coinciding with the region R. Of course, (2.5) and (2.6) provide equivalent statements of mass conservation. *That these hold for arbitrary regions of macroscopic proportion implies they hold for any arbitrarily small rectangular box*—the integral over such is expressible in terms of integrals over (eight) macroscopic boxes. Hence, by continuity, the local forms follow. In particular,

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0.$$

An immediate consequence is Reynolds' transport theorem (cf. (**12**), §81)

$$\frac{d}{dt}\int_{R_t} \rho f = \int_{R_t} \rho \dot{f}, \tag{2.7}$$

for any C^1-function f definition the trajectory of the body.

3. Non-thermodynamic balance relations for solids

3.1. *Linear momentum*

The net force exerted upon particle P_i is supposed at any instant to be attributable to individual interactions with all other particles, $\mathbf{f}_{il}$ denoting that force exerted by P_l, together with an external force per unit mass $\mathbf{b}_i$. (Of course, $\mathbf{f}_{il}$ may depend upon the positions, velocities etc. of all other particles at this stage.) If P_i exerts no force on itself its motion is governed by

$$\sum_{l \neq i} \mathbf{f}_{il} + m_i \mathbf{b}_i = d/dt(m_i \mathbf{v}_i). \tag{3.1}$$

Let R be a macroscopic region within that region occupied by the body and consider the sum of equations (3.1) with P_i in R. Defining $\mathbf{b}$ by

$$\mathbf{b} := \lim_{\varepsilon} \{\mathbf{b}_\varepsilon\}, \quad \text{where} \quad \mathbf{b}_\varepsilon := \sum_i{}' m_i \mathbf{b}_i \Big/ \sum_i{}' m_i \tag{3.2}$$

in the now familiar ε-cell sense (here and in what follows sums over such cells will be distinguished by a superposed prime) implies the net external (or body) force acting upon R is

$$\int_R \rho \mathbf{b}.$$

Similarly, the corresponding sum over P_i in R

$$\sum_i d/dt(m_i \mathbf{v}_i) = d/dt\left(\sum_i m_i \mathbf{v}_i\right) \tag{3.3}$$

is to be identified with

$$\frac{d}{dt}\int_{R_t} \rho \mathbf{v},$$

R_t (cf. (2.6)) appearing by virtue of a fixed set of particles being intended in (3.3).

The remaining double sum $\sum\sum_{i\neq l} \mathbf{f}_{il}$ decomposes naturally into two parts, one of which involves pairs of particles both of which lie in R, the other pairs in which just one particle lies in R. Denoting these by $\sum\sum_{i\neq k} \mathbf{f}_{ik}$ and $\sum_i\sum_j \mathbf{f}_{ij}$ respectively, we assume that

$$\sum\sum_{i\neq k} \mathbf{f}_{ik} = \mathbf{0}. \tag{3.4}$$

Since this expression may be written in the form

$$\tfrac{1}{2}\sum\sum_{i\neq k} (\mathbf{f}_{ik} + \mathbf{f}_{ki}),$$

this postulate is clearly consistent with the much stronger assumption that $(\mathbf{f}_{ik} + \mathbf{f}_{ki})$ should vanish for each pair P_i, P_k. Statement (3.4) merely requires that the net self-force of any set of particles within a macroscopic region R should vanish. (If R is broken up into two disjoint macroscopic regions R_1 and R_2, then the foregoing assumption readily implies that the net force exerted by particles in R_1 upon those in R_2 is equal and opposite to that exerted by particles in R_2 upon those in R_1. That is, assumption (3.4) gives rise to Newton's third law at the macroscopic level.)

In treating the remaining sum the crucial assumption that interactions be essentially local is made. (Remarks on non-local interaction (as, for example, that due to gravitation) are made in section 5.) More precisely, it is assumed that the net force on an individual particle, P_i say, due to its interactions with *all* other particles is given by

$$\sum_{l\neq i} \mathbf{f}_{il} = \sum_{m\neq i} \mathbf{f}_{im}, \quad \text{where} \quad P_iP_m < \delta \ll 10^{-5}\text{m}. \tag{3.5}$$

(For definiteness we take $\delta = 1000\ \text{Å} = 10^{-7}$ m.)

This is much weaker than the assumption

$$\mathbf{f}_{il} = \mathbf{0} \quad \text{for} \quad P_iP_l \geq \delta,$$

admitting *individual* interactions of much greater effective range than 1000 Å. Here we have in mind ion–ion interactions, (3.5) resulting from judicious book-keeping in balancing the forces on P_i due to ions of opposite net charge at distances in excess of δ. It follows that the only contributions to $\sum_i\sum_j \mathbf{f}_{ij}$ arise from interactions between particles within inner and outer "δ-envelopes" of ∂R; that is, regions bounded by ∂R and parallel surfaces distant δ therefrom, lying inside and outside R respectively. Let $\mathbf{x}\in\partial R$ and consider the sum $\sum_i{\sum_j}' \mathbf{f}_{ij}$ taken over particles within an ε-cell centred at $\mathbf{x}$, $C_\varepsilon(\mathbf{x})$ say. The above remarks imply that this sum essentially involves only particles P_i in a cylindrical region of cross-section $C_\varepsilon(\mathbf{x}) \cap \partial R$ with height

10^{-7} m. Such particles are said to form an *ε-surface cell centred at* $\mathbf{x}$. We define

$$\mathbf{t}_\varepsilon(\mathbf{x}, t) := \sum_i \sum_j{}' \mathbf{f}_{ij} \Big/ A_\varepsilon,$$

where

$$A_\varepsilon := \text{Area}\,(C_\varepsilon(\mathbf{x}) \cap \partial R),$$

and, if it exists,

$$\mathbf{t}(\mathbf{x}, t) := \lim_\varepsilon \{\mathbf{t}_\varepsilon(\mathbf{x}, t)\}. \tag{3.6}$$

Of course, $\mathbf{t}$ is the traction field on ∂R, and the continuum version of the total sum $\sum_i \sum_j \mathbf{f}_{ij}$ is

$$\int_{\partial R} \mathbf{t}.$$

Although $\mathbf{t}$ as here defined might be expected to be sensitive to fluctuations (cf. Alblas (**14**), p. 281) discussion of this is postponed until section 4. See also Korotkina (**15**) for the statistical viewpoint.

It follows from the foregoing that summation of individual equations of motion for particles in R yields

$$\int_{\partial R} \mathbf{t} + \int_R \rho\mathbf{b} = \frac{d}{dt} \int_{R_t} \rho\mathbf{v} = \int_R \rho\mathbf{a}, \tag{3.7}$$

the second equality following from (2.7). (Consequently $\mathbf{a}$ may be defined alternatively as $\lim_\varepsilon \{\mathbf{a}_\varepsilon\}$, where $\mathbf{a}_\varepsilon := \sum_i{}' m_i \mathbf{a}_i / \sum_i{}' m_i$ with $\mathbf{a}_i := d\mathbf{v}_i/dt$.) It is now possible in the usual way to exhibit the existence of the stress tensor $\mathbf{T}$ upon assuming $\mathbf{t}$ to be a continuous function of position and orientation: definition (3.6) makes such assumptions plausible. With $\mathbf{n}$ denoting the outward unit normal to ∂R, so that $\mathbf{t} = \mathbf{Tn}$, equation (3.7) implies that if $\mathbf{T}$ is sufficiently smooth,

$$\int_R (\text{div}\,\mathbf{T} + \rho\mathbf{b} - \rho\mathbf{a}) = \mathbf{0}$$

for all macroscopic regions R and thus, since integrals are additive over arbitrary disjoint regular regions, for *all* regions. Hence, by continuity,

$$\text{div}\,\mathbf{T} + \rho\mathbf{b} = \rho\mathbf{a} \tag{3.8}$$

at all points occupied by the body.

3.2. *Generalised moment of momentum*

If the terms of (3.1) are tensorially pre-multiplied† by $(\mathbf{x}_i - \mathbf{x}_0)$, where $\mathbf{x}_i$ denotes the instantaneous location of P_i and $\mathbf{x}_0$ is an arbitrary geometrical

† Recall $(\mathbf{a}\otimes\mathbf{b})\mathbf{c} := (\mathbf{b} \cdot \mathbf{c})\mathbf{a}$ for any vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$. Equivalently $(\mathbf{a}\otimes\mathbf{b})_{ij} = a_i b_j$.

point, and summed over all P_i in R, then the external force contribution to this sum from an ε-cell in R is

$$\sum_i{}'(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{b}_i=\sum_i{}'(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i(\mathbf{b}_i-\mathbf{b}_\varepsilon)+(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes\left(\sum_i{}'m_i\right)\mathbf{b}_\varepsilon, \tag{3.9}$$

where $\mathbf{x}_\varepsilon$ denotes the mass centre of those particles within the cell and $\mathbf{b}_\varepsilon$ is defined by $(3.2)_2$. In this decomposition the latter term gives rise to a total contribution from within R of

$$\int_R(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{b}, \tag{3.10}$$

while the first sum must in general be expected to be negligible compared with the second. More precisely, if the external force derives from a field $\hat{\mathbf{b}}$ everywhere defined (for example, gravitation, when $\mathbf{b}_i$ is the gravitational acceleration at $\mathbf{x}_i$ due to matter outside the body) and of class C^1, then it is a simple matter to show that $\mathbf{b}_\varepsilon=\hat{\mathbf{b}}(\mathbf{x}_\varepsilon)$ to within order $o(\varepsilon)$, so that

$$\mathbf{b}_i-\mathbf{b}_\varepsilon=\nabla\hat{\mathbf{b}}(\mathbf{x}_\varepsilon)(\mathbf{x}_i-\mathbf{x}_\varepsilon)+o(\varepsilon).$$

Hence

$$\sum_i{}'(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i(\mathbf{b}_i-\mathbf{b}_\varepsilon)=\mathbf{I}(\nabla\hat{\mathbf{b}})^T+\left(\sum_i{}'m_i\right)o(\varepsilon^2),$$

where

$$\mathbf{I}:=\sum_i{}'(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i(\mathbf{x}_i-\mathbf{x}_\varepsilon). \tag{3.11}$$

Since $\|\mathbf{x}_i-\mathbf{x}_\varepsilon\|<2\varepsilon$,

$$\|\mathbf{I}\|<4\varepsilon^2\sum_i{}'m_i,$$

so that the contributions to (3.9) from the two sums have orders of magnitude in the ratio $\varepsilon^2\|\nabla\hat{\mathbf{b}}\|:\|\mathbf{x}-\mathbf{x}_0\|\,.\,\|\hat{\mathbf{b}}\|$.

It is useful in making estimates as above to assume that particles within any given ε-cell deform homogeneously with time (this is felt to be a realistic approximation for solids but quite inappropriate for fluids): that is,

$$\mathbf{x}_i(t)-\mathbf{x}_k(t)=\mathbf{F}(t)(\hat{\mathbf{x}}_i-\hat{\mathbf{x}}_k), \tag{3.12}$$

where $\mathbf{F}(t)$ is an invertible linear map, and $\mathbf{x}_i(t)$ $(\mathbf{x}_k(t))$ and $\hat{\mathbf{x}}_i(\hat{\mathbf{x}}_k)$ denote the location of $P_i(P_k)$ at instants t and $\hat{t}$ respectively. In such case (3.11) may be written as

$$\mathbf{I}=\mathbf{F}\hat{\mathbf{I}}\mathbf{F}^T, \tag{3.13}$$

where

$$\hat{\mathbf{I}}:=\sum_i{}'(\hat{\mathbf{x}}_i-\hat{\mathbf{x}}_\varepsilon)\otimes m_i(\hat{\mathbf{x}}_i-\hat{\mathbf{x}}_\varepsilon),$$

$\hat{\mathbf{x}}_\varepsilon$ denoting the mass centre of the cell (it is to be noted that homogeneous

motions preserve mass centres) at instant t. Clearly the ratio of $\hat{\mathbf{I}}$ to the mass within the cell is of order $O(\varepsilon^2)$. (Here we are implicitly assuming $\mathbf{F}$ is of order $O(1)$.)

The contribution from mass acceleration terms within an ε-cell may be written as

$$\sum_i{}'(\mathbf{x}_i-\mathbf{x}_0)\otimes d/dt(m_i\mathbf{v}_i)=d/dt\left\{\sum_i{}'(\mathbf{x}_i-\mathbf{x}_e)\otimes m_i(\mathbf{v}_i-\mathbf{v}_e)+\right.$$
$$\left.+(\mathbf{x}_e-\mathbf{x}_0)\otimes\left(\sum_i{}'m_i\right)\mathbf{v}_e\right\}$$
$$-\sum_i{}'(\mathbf{v}_i-\mathbf{v}_e)\otimes m_i(\mathbf{v}_i-\mathbf{v}_e)-\mathbf{v}_e\otimes\left(\sum_i{}'m_i\right)\mathbf{v}_e,$$

where $\mathbf{v}_e$ is defined by $(2.3)_2$. The terms involving $\mathbf{x}_i$ and $\mathbf{v}_i$ are readily shown to be negligible on assuming (3.12):

$$\sum_i{}'(\mathbf{x}_i-\mathbf{x}_e)\otimes m_i(\mathbf{v}_i-\mathbf{v}_e)=\mathbf{F}\hat{\mathbf{I}}\dot{\mathbf{F}}^T$$

and

$$\sum_i{}'(\mathbf{v}_i-\mathbf{v}_e)\otimes m_i(\mathbf{v}_i-\mathbf{v}_e)=\dot{\mathbf{F}}\hat{\mathbf{I}}\dot{\mathbf{F}}^T$$

have time derivatives of order $\left(\sum_i{}'m_i\right)\varepsilon^2$ (on assuming $\|\mathbf{F}\|$, $\|\dot{\mathbf{F}}\|$, and $\|\ddot{\mathbf{F}}\|$ are $O(1)$). The remaining terms give rise to a contribution from R of

$$\frac{d}{dt}\left\{\int_{R_t}(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{v}\right\}-\int_R\mathbf{v}\otimes\rho\mathbf{v}. \tag{3.14}$$

The sum involving interactions decomposes as in section 3.1:

$$\sum_i(\mathbf{x}_i-\mathbf{x}_0)\otimes\sum_{l\neq i}\mathbf{f}_{il}=\sum_i(\mathbf{x}_i-\mathbf{x}_0)\otimes\sum_{k\neq i}\mathbf{f}_{ik}+\sum_i(\mathbf{x}_i-\mathbf{x}_0)\otimes\sum_j\mathbf{f}_{ij}$$
$$=\mathbf{J}_{\text{tot}}+\mathbf{S},\quad\text{say.} \tag{3.15}$$

By virtue of assumption (3.4), $\mathbf{J}_{\text{tot}}$ is independent of $\mathbf{x}_0$ and so represents an intrinsic tensorial parameter associated with the particles within R. If $\mathbf{f}_{ik}$ is parallel to $(\mathbf{x}_i-\mathbf{x}_k)$ and $(\mathbf{f}_{ik}+\mathbf{f}_{ki})$ zero for all P_i, P_k, then $\mathbf{J}_{\text{tot}}$ is easily shown to be symmetric. More generally, the skew part of $\mathbf{J}_{\text{tot}}$ is the self-couple associated with these particles. We assume that such a self-couple (namely, that associated with particles in a macroscopic region) is zero, or, equivalently, that

$$\mathbf{J}_{\text{tot}}\text{ is symmetric.} \tag{3.16}$$

The only non-zero contribution to $\mathbf{S}$ derives, by virtue of (3.5), from interactions between the inner and outer 'δ-envelopes' centred on ∂R as

introduced in subsection 3.1. As therein, let $\mathbf{x}\in\partial R$ and consider the contribution from particles in an ε-surface cell centred at $\mathbf{x}$, namely

$$\sum_i \sum_j{}' (\mathbf{x}_i-\mathbf{x})\otimes\mathbf{f}_{ij}+(\mathbf{x}-\mathbf{x}_0)\otimes\sum_i\sum_j{}'\mathbf{f}_{ij}.$$

While the second term has continuum counterpart for the total sum

$$\int_{\partial R}(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{t}, \tag{3.17}$$

the first term may be regarded as a local measure of uneven particle distribution (or inhomogeneity). If, upon dividing by the cross-sectional surface cell area, this first term is of order $O(\varepsilon^2)$, then (3.10), (3.14), (3.15) and (3.17) imply that

$$\mathbf{J}_{\text{tot}}+\int_{\partial R}(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{t}+\int_R(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{b}=d/dt\left\{\int_{R_t}(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{v}\right\}-\int_R\rho\mathbf{v}\otimes\mathbf{v}, \tag{3.18}$$

upon neglecting $O(\varepsilon^2)$-terms. By virtue of (3.16) the skew part of (3.18) yields the classical form of rotational momentum balance:

$$\int_{\partial R}(\mathbf{x}-\mathbf{x}_0)\wedge\mathbf{t}+\int_R(\mathbf{x}-\mathbf{x}_0)\wedge\rho\mathbf{b}=d/dt\left\{\int_{R_t}(\mathbf{x}-\mathbf{x}_0)\wedge\rho\mathbf{v}\right\}. \tag{3.19}$$

(Here we recall that

$$\mathbf{a}\wedge\mathbf{b}:=\mathbf{a}\otimes\mathbf{b}-(\mathbf{a}\otimes\mathbf{b})^{\mathrm{T}}=\mathbf{a}\otimes\mathbf{b}-\mathbf{b}\otimes\mathbf{a}$$

has axial vector $-\mathbf{a}\times\mathbf{b}$.)

In the event that

$$\lim_{\varepsilon}\left\{\sum_i\sum_j{}'(\mathbf{x}_i-\mathbf{x})\otimes\mathbf{f}_{ij}\Big/A_\varepsilon\right\}=:\mathbf{C}^+$$

makes sense and is not negligible, (3.18) and (3.19) must be modified: the surface integrals in such case have integrands $(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{t}+\mathbf{C}^+$ and $(\mathbf{x}-\mathbf{x}_0)\wedge\mathbf{t}+\mathbf{C}$ respectively, where $\mathbf{C}$ denotes the skew part of $\mathbf{C}^+$.

3.3. *Energy*

Scalar multiplication of (3.1) by $\mathbf{v}_i$ followed by summation of the resulting equations for all P_i in R yields

$$\sum_{i\neq l}\sum_l\mathbf{f}_{il}\cdot\mathbf{v}_i+\sum_i m_i\mathbf{b}_i\cdot\mathbf{v}_i=\sum_i m_i\mathbf{a}_i\cdot\mathbf{v}_i=d/dt\left\{\sum_i\tfrac{1}{2}m_i\mathbf{v}_i^2\right\}. \tag{3.20}$$

In the manner of the preceding subsection, the second and third terms give rise, upon neglect of order $O(\varepsilon^2)$-terms, to continuum counterparts

$$\int_R\rho\mathbf{b}\cdot\mathbf{v}\quad\text{and}\quad d/dt\left\{\int_{R_t}\tfrac{1}{2}\rho\mathbf{v}^2\right\}, \tag{3.21}$$

respectively. The neglected terms are, at the ε-cell level and upon using (3.12), respectively, $\nabla\hat{\mathbf{b}}.\dot{\mathbf{F}}\hat{\mathbf{I}}\mathbf{F}^T$ and $\hat{\mathbf{I}}.\dot{\mathbf{F}}^T\ddot{\mathbf{F}}$. (If $\mathbf{A}$ and $\mathbf{B}$ are linear transformations then $\mathbf{A}.\mathbf{B} := \text{trace}\,(\mathbf{A}^T\mathbf{B}) = A_{ij}B_{ij}$.) The first term of (3.20) decomposes into surface and volume contributions, the former of which gives rise to a sum over surface cells of terms

$$\sum_i \sum_j{}' \mathbf{f}_{ij}.\mathbf{v}_i = \sum_i \sum_j{}' \mathbf{f}_{ij}.\mathbf{v}_e + \sum_i \sum_j{}' \mathbf{f}_{ij}.(\mathbf{v}_i - \mathbf{v}_e). \tag{3.22}$$

Adopting (3.12), the third term may be written as

$$\sum_i \sum_j{}' \mathbf{f}_{ij}.\mathbf{L}(\mathbf{x}_i - \mathbf{x}_e) = \left(\sum_i \sum_j{}' (\mathbf{x}_i - \mathbf{x}_e)\otimes\mathbf{f}_{ij}\right).\mathbf{L}^T,$$

where $\mathbf{L} := \dot{\mathbf{F}}/\mathbf{F}^{-1}$. Neglect of this term is thus consistent with (3.18), while if (3.18) is augmented by the surface integral of $\mathbf{C}^+$ over ∂R then the energy balance contains the surface integral of $\mathbf{C}^+.\mathbf{L}^T$ over ∂R on assuming that $\|\mathbf{x}-\mathbf{x}_e\|$ is of order $O(\varepsilon^2)$. Of course, the middle term of (3.22) gives rise to a total sum respresented by

$$\int_{\partial R} \mathbf{t}.\mathbf{v}. \tag{3.23}$$

The volume contribution from the first term of (3.20), namely $\sum_{i\neq k}\sum \mathbf{f}_{ik}.\mathbf{v}_i$, admits of simple interpretation when interactions are delivered by separation-dependent pair-potentials; that is,

$$\mathbf{f}_{ik} = \alpha_{ik}(\|\mathbf{x}_i - \mathbf{x}_k\|^2)(\mathbf{x}_i - \mathbf{x}_k). \tag{3.24}$$

In such case, the work done in bringing P_i to its current location from infinite dispersion in the presence of all other particles located at their current positions is, from the strictly pairwise nature of such interactions, $\sum_{k\neq i} w_{ik}$, where

$$w_{ik} := \int_r^\infty \alpha_{ik}(s^2)s\,ds,$$

with

$$r := \|\mathbf{x}_i(t) - \mathbf{x}_k(t)\|.$$

Clearly we have

$$\dot{w}_{ik} = -\mathbf{f}_{ik}.(\mathbf{v}_i - \mathbf{v}_k).$$

Since the total work done in assembling the particles from a state of infinite dispersion is

$$W_{\text{tot}} := \tfrac{1}{2}\sum_{i\neq k}\sum w_{ik},$$

and, for the interactions considered, $\mathbf{f}_{ik} + \mathbf{f}_{ki} = \mathbf{0}$, it follows that

$$a := -\sum_{i\neq k}\sum \mathbf{f}_{ik}.\mathbf{v}_i = -\tfrac{1}{2}\sum_{i\neq k}\sum \mathbf{f}_{ik}.(\mathbf{v}_i - \mathbf{v}_k) = \tfrac{1}{2}\sum_{i\neq k}\sum \dot{w}_{ik} = \dot{W}_{\text{tot}}. \tag{3.25}$$

That is, the volume contribution is to be identified with the time rate of change of the binding energy of the particles within R when interactions take the form of (3.24).

$$\dot{w} := -\lim_{\varepsilon}\left\{\sum_{i}\sum_{k}{}' \mathbf{f}_{ik}\cdot\mathbf{v}_i \Big/ \sum_{i}{}' m_i\right\}, \tag{3.26}$$

(so that w is essentially the binding energy per unit mass for an ε-cell) and dividing R up into such cells yields

$$a = \dot{W}_{\text{tot}} = \frac{d}{dt}\int_{R_t}\rho w = \int_R \rho\dot{w} \tag{3.27}$$

if the binding energies associated with interactions between cells are neglected. This we regard as reasonable and consistent with the assumption $\delta \ll \varepsilon$ (cf. (3.5)).

An alternative expression for the foregoing sum is available if the net self-force of particles within ε-cells is assumed to vanish $\left(\text{so that } \sum_{i}\sum_{k}{}' (\mathbf{x}_i - \mathbf{x}_0)\otimes\mathbf{f}_{ik}\right.$ taken over such a cell is independent of $\left.\mathbf{x}_0\right)$ and

$$\mathbf{J} := \lim_{\varepsilon}\left\{\sum_{i}\sum_{k}{}' (\mathbf{x}_i - \mathbf{x}_0)\otimes\mathbf{f}_{ik}\Big/ V_\varepsilon\right\} = \lim_{\varepsilon}\left\{\sum_{i}\sum_{k}{}' (\mathbf{x}_i - \mathbf{x}_\varepsilon)\otimes\mathbf{f}_{ik}\Big/ V_\varepsilon\right\} \tag{3.28}$$

is meaningful. *In such case we feel that consistent with the assumed vanishing of the self-force associated with an ε-cell is that also of the self-couple. Thus we assume* $\mathbf{J}$ *symmetric if it exists.* Assuming contributions to $\mathbf{J}_{\text{tot}}$ (cf. (3.15)) from interactions between cells is negligible,

$$\mathbf{J}_{\text{tot}} = \int_R \mathbf{J}. \tag{3.29}$$

Further, within each cell (assuming locally homogeneous deformation)

$$\mathbf{v}_i = \mathbf{v}_\varepsilon + \mathbf{L}(\mathbf{x}_i - \mathbf{x}_\varepsilon)$$

so that

$$\sum_{i}\sum_{k}{}' \mathbf{f}_{ik}\cdot\mathbf{v}_i = \left(\sum_{i}\sum_{k}{}' (\mathbf{x}_i - \mathbf{x}_\varepsilon)\otimes\mathbf{f}_{ik}\right).\mathbf{L}^T. \tag{3.30}$$

It follows from (3.25), (3.28) and (3.30), that

$$a = \sum_{i}\sum_{k}\mathbf{f}_{ik}\cdot\mathbf{v}_i = -\int_R \mathbf{J}.\mathbf{L}^T = -\int_R \mathbf{J}.\mathbf{D}, \tag{3.31}$$

where $\mathbf{D}$ is the symmetric part of $\mathbf{L}$.

Thus the continuum version of (3.20) is, upon neglecting $O(\varepsilon^2)$-terms and couple stress,

$$\int_{\partial R}\mathbf{t}.\mathbf{v} + \int_R \rho\mathbf{b}.\mathbf{v} = a + d/dt\left\{\int_{R_t}\tfrac{1}{2}\rho\mathbf{v}^2\right\} \tag{3.32}$$

upon using (3.21) and (3.23), a being given by (3.27) or (3.31) as appropriate (we remark that these alternatives are not mutually exclusive).

3.4. *Remarks*

3.4.1. Writing $\mathbf{t}=\mathbf{Tn}$ and utilising (3.29) and (3.8), the local form of (3.18) is

$$\mathbf{T}^T+\mathbf{J}=\mathbf{0}.$$

That is, $\mathbf{T}$ is symmetric and $\mathbf{J}$ is to be identified with $-\mathbf{T}$. Further, the local form of (3.32), upon using (3.31) and (3.8), is

$$\mathbf{T}.\nabla\mathbf{v}=-\mathbf{J}.\mathbf{D}$$

so that

$$\mathbf{T}.\tfrac{1}{2}(\nabla\mathbf{v}+\nabla\mathbf{v}^T)=\mathbf{T}.\mathbf{D}.$$

Of course, this is consistent with $\mathbf{F}$ (as introduced in (3.12)) being the deformation gradient of the motion relative to the configuration existing at instant $\hat{t}$ in which case $\mathbf{L}=\nabla\mathbf{v}$. Indeed, it is difficult to see how $\mathbf{F}$ might otherwise have been interpreted.

3.4.2. It is tempting to try to incorporate the neglected terms in the previous two subsections within the balance relations by utilising their relationships with $\mathbf{F}$, $\dot{\mathbf{F}}$ and $\hat{\mathbf{I}}$. However, we cannot expect $\lim_\varepsilon\{\hat{\mathbf{I}}\}$ to exist (essentially micro*structure* is needed for this purpose) since the sum involved is highly sensitive both to the geometry of cells used and their size. Our purpose in (3.13) was merely to introduce a quantity, namely $\hat{\mathbf{I}}$, which emphasised the $O(\varepsilon^2)$-nature of the aforementioned terms.

3.4.3. Considerations of frame-indifference for the particles readily lead to the usual requirements for continuum parameters (cf. (**1**, §19)). For example, in a frame change in which

$$\mathbf{x}\to\mathbf{x}^*=\mathbf{c}+\mathbf{Q}(\mathbf{x}-\mathbf{x}_0), \tag{3.33}$$

$\mathbf{c}$ and $\mathbf{Q}$ being point- and proper orthogonal-valued functions of time respectively, the velocity of P_i transforms as

$$\mathbf{v}_i\to\mathbf{v}_i^*=\dot{\mathbf{c}}+\dot{\mathbf{Q}}(\mathbf{x}_i-\mathbf{x}_0)+\mathbf{Q}\mathbf{v}_i.$$

Thus, from (2.3), $\mathbf{v}_\varepsilon$ transforms as

$$\mathbf{v}_\varepsilon\to\mathbf{v}_\varepsilon^*=\dot{\mathbf{c}}+\dot{\mathbf{Q}}(\mathbf{x}_\varepsilon-\mathbf{x}_0)+\mathbf{Q}\mathbf{v}_\varepsilon,$$

so that the continuum velocity field transforms as

$$\mathbf{v}\to\mathbf{v}^*=\dot{\mathbf{c}}+\dot{\mathbf{Q}}(\mathbf{x}-\mathbf{x}_0)+\mathbf{Q}\mathbf{v}$$

to within the order of terms neglected in the previous subsections if we assume $\lim_\varepsilon\{\mathbf{x}_\varepsilon-\mathbf{x}\}=O(\varepsilon^2)$. Similarly, under the same assumption,

$$\mathbf{a}\to\mathbf{a}^*=\ddot{\mathbf{c}}+\ddot{\mathbf{Q}}(\mathbf{x}-\mathbf{x}_0)+2\dot{\mathbf{Q}}\mathbf{v}+\mathbf{Q}\mathbf{a}.$$

Clearly the assumption that individual interactions $\mathbf{f}_{il}$ are frame-indifferent (that is, $\mathbf{f}_{il} \to \mathbf{Q}\mathbf{f}_{il}$, as is trivially the case for interactions (3.24)) implies that $\mathbf{t} \to \mathbf{Q}\mathbf{t}$, $\mathbf{C}^+ \to \mathbf{Q}\mathbf{C}^+\mathbf{Q}^T$, $\mathbf{J} \to \mathbf{Q}\mathbf{J}\mathbf{Q}^T$, and $a \to a$.

3.4.4. Following Green and Rivlin (cf. (**16**)) it is common practice to derive balances of linear and rotational momentum from a postulated energy balance together with the assumption that such be invariant under superposed rigid motions (equivalently, frame-indifferent (cf. Murdoch (**17**)). As demonstrated in subsection 3.3, energy balance derives from the sum of equations of motion for individual particles when scalarly multiplied by the velocities of these particles. Since

$$\sum_{l \neq i} \mathbf{f}_{il} + m_i(\mathbf{b}_i - \mathbf{a}_i) = \mathbf{0},$$

it follows that

$$\mathbf{Q}\left(\sum_{l \neq i} \mathbf{f}_{il} + m_i(\mathbf{b}_i - \mathbf{a}_i)\right).(\dot{\mathbf{c}} + \dot{\mathbf{Q}}(\mathbf{x}_i - \mathbf{x}_0) + \mathbf{Q}\mathbf{v}_i) = 0 \tag{3.34}$$

for all frame changes (3.33). That is,

$$\left(\sum_{l \neq i} \mathbf{f}_{il}^* + m_i(\mathbf{b}_i^* - \mathbf{a}_i^*)\right).\mathbf{v}_i^* = 0,$$

whence the energy balance appropriate to the new frame is obtained by summation. That is, *the energy equation is invariant under changes of frame.* (Here $\mathbf{a}_i^*$ denotes the acceleration in the new frame. Thus $\mathbf{b}_i^* \neq \mathbf{Q}\mathbf{b}_i$ and $\mathbf{a}_i^* \neq \mathbf{Q}\mathbf{a}_i$ but $\mathbf{b}_i^* - \mathbf{a}_i^* = \mathbf{Q}(\mathbf{b}_i - \mathbf{a}_i)$, and $\mathbf{b}_i^* - \mathbf{Q}\mathbf{b}_i$ is given by the inertial terms which comprise the mismatch between $\mathbf{a}_i^*$ and $\mathbf{Q}\mathbf{a}_i$.)

4. Naïve thermodynamics

4.1. *Basic concepts and linear momentum balance*

In the foregoing no account has been taken of possible fluctuations in the values (that is, significant but erratic changes in these values which take place on a microscopic time scale) of physical parameters due to the chaotic (thermal) motions of individual particles. To accommodate thermal considerations we define, in respect of a physical parameter φ,

$$\varphi_\Delta(t) := \frac{1}{\Delta}\int_{t-\Delta}^{t} \varphi(\tau)\, d\tau. \tag{4.1}$$

In what follows it will be assumed for certain parameters φ that $\varphi_\Delta(t)$ is insensitive to Δ-values corresponding to macroscopically small yet microscopically large time intervals. (For example, intervals of order 10^{-7} sec. are appropriate for crystals, the time scale for molecular vibrations therein being of order 10^{-12} sec.) The Δ-insensitive value in question, hereafter denoted by $\bar{\varphi}(t)$, is, of course, the temporal counterpart of the spatial "ε-limit"

already introduced. The *fluctuation* φ' in φ is given by

$$\varphi' := \varphi - \bar{\varphi}.$$

For the parameters concerned $\bar{\varphi}(t)$ will be assumed to vary negligibly over macroscopically small time intervals; more precisely, for parameters φ and ψ it will be assumed that

$$\left.\begin{aligned} \bar{\bar{\varphi}} = \bar{\varphi} \qquad & (\text{equivalently } \bar{\varphi}' = 0), \\ \overline{\bar{\varphi}\bar{\psi}} = \bar{\varphi}\bar{\psi} \quad \text{and} \quad & \overline{\bar{\varphi}\psi'} = 0. \end{aligned}\right\} \tag{4.2}$$

A simple consequence of (4.1) is that

$$\dot{\bar{\varphi}} = \bar{\dot{\varphi}}, \tag{4.3}$$

while $(4.2)_2$ and $(4.2)_3$ imply that

$$\overline{\varphi\psi} = \bar{\varphi}\bar{\psi} + \overline{\varphi'\psi'}. \tag{4.4}$$

The basic definitions of sections 2 and 3 are now modified somewhat. The quantities ρ and $\mathbf{v}$ as given by (2.1), (2.2), and (2.3) are assumed free of fluctuation; that is, although over a Δ-time interval a spatially fixed ε-cell will contain a changing particle population, ρ and $\mathbf{v}$ defined thereby will vary only in macroscopic fashion (that is, change appreciably only over time intervals considerably in excess of Δ). Now consider a macroscopic region R divided up into ε-cells and its δ-collared boundary region divided up into ε-surface cells. The images of R and these cells under the motion $\boldsymbol{\chi}$ defined in terms of $\mathbf{v}$ by (2.4) will, for each instant τ in the time interval $[t-\Delta, t]$, yield a macroscopic region R_τ together with ε-cells therein.

The body-force field $\mathbf{b}$ is now defined at instant t by (cf. (3.2))

$$\mathbf{b} := \lim_\varepsilon \left\{ \overline{\sum_i{}' m_i \mathbf{b}_i} \Big/ \overline{\sum_i{}' m_i} \right\},$$

where the sum is over a deforming ε-cell as described above. Since the cell deforms with the body, the sum will involve essentially the same particles throughout the Δ-time interval. Consequently we may write

$$\overline{\sum_i{}' m_i \mathbf{b}_i} = \sum_i{}' m_i \bar{\mathbf{b}}_i \quad \text{and} \quad \overline{\sum_i{}' m_i} = \sum_i{}' m_i =: m_\varepsilon.$$

The traction field is similarly defined (on $\partial R = \partial R_t$) by (cf. (3.6))

$$\mathbf{t} := \lim_\varepsilon \left\{ \overline{\sum_i \sum_j{}' \mathbf{f}_{ij}} \Big/ A_\varepsilon \right\}, \tag{4.5}$$

noting that it is not necessary to invoke a time-averaged denominator since its variation over a Δ-interval is negligible. However, the double sum in (4.5) most definitely does *not* involve the same particles at all instants in the Δ-interval.

At any instant τ, as in section 3,

$$\sum_i \sum_j \mathbf{f}_{ij} + \sum_i m_i \mathbf{b}_i = d/dt \left\{ \sum_i m_i \mathbf{v}_i \right\},$$

the sums being over P_i inside R_τ and P_j outside R_τ. On taking the time average over $[t-\Delta, t]$ and using (4.5) and (4.3), the continuum version is seen to be

$$\int_{\partial R} \mathbf{t} + \int_R \rho \mathbf{b} = \frac{d}{dt} \int_{R_t} \rho \mathbf{v}.$$

That is, the *form* of linear momentum balance is unchanged on taking thermal motion into account. What have changed, of course, are the definitions of $\mathbf{t}$ and $\mathbf{b}$, these quantities now being local averages in time as well as space.

Before proceeding further it is necessary, within the simplistic particle model here utilised, to address the fundamental difference in the nature of thermal motion as manifested in solid and fluid phases. Roughly speaking, particles in a solid phase undergo chaotic motions of small amplitude about points which move in a manner commensurate with the local macroscopic motion, while those in a fluid phase describe Brownian-type trajectories.

More precisely, for a particle P_i in a solid phase it will be assumed that $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{v}}_i$ are well-defined, $\mathbf{x}_i'$ being of order $O(\varepsilon^2)$, and that for any ε-cell ($\varepsilon \sim 10^{-5}$ m)

S.1. $$\bar{\mathbf{v}}_i = \mathbf{v}(\mathbf{x}_\varepsilon) + \mathbf{L}(\bar{\mathbf{x}}_i - \mathbf{x}_\varepsilon), \quad \text{where} \quad \mathbf{L} := \nabla \mathbf{v}(\mathbf{x}_\varepsilon),$$

S.2. $$\sum_i{}' m_i \mathbf{x}_i' = \mathbf{0},$$

and S.3. $$\sum_i{}' \overline{\mathbf{x}_i' \otimes m_i \mathbf{v}_i'} = \mathbf{0}.$$

It follows from S.2. that

$$\sum_i{}' m_i (\bar{\mathbf{x}}_i - \mathbf{x}_\varepsilon) = \mathbf{0}, \tag{4.6}$$

(so that $\mathbf{x}_\varepsilon$ is not subject to fluctuation) and the fluctuation-free nature of $\mathbf{v}_\varepsilon$ implies

$$\sum_i{}' m_i \mathbf{v}_i' = \mathbf{0}, \quad \text{whence} \quad \mathbf{v}(\mathbf{x}_\varepsilon) = \mathbf{v}_\varepsilon, \tag{4.7}$$

on using S.1. and (4.6).

If P_i is in a fluid phase ($\bar{\mathbf{x}}_i$ in such case being meaningless) then it will be assumed for ε-cells as above that

F.1. $$\sum_i{}' \overline{(\mathbf{x}_i - \mathbf{x}_\varepsilon) \otimes m_i (\mathbf{v}_i - \mathbf{v}_\varepsilon)} = \mathbf{0}$$

and

F.2. $\mathbf{x}_\varepsilon$ is not subject to fluctuation.

4.2. *Generalised moment of momentum balance*

As in section 3, tensorial pre-multiplication of the equation of motion of a typical particle by its instantaneous displacement from an arbitrary point $\mathbf{x}_0$ yields, on summing over all particles in a macroscopic region R,

$$\sum_{i}\sum_{l\neq i}(\mathbf{x}_i-\mathbf{x}_0)\otimes\mathbf{f}_{il}+\sum_i(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{b}_i=\sum_i(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\,d\mathbf{v}_i/dt.$$

The relationship sought is the continuum version of the Δ-time average of this relationship.

The body-force contribution from an ε-cell within R is, noting $\mathbf{x}_\varepsilon$ is fluctuation-free and using (4.4),

$$\sum_i{}'\overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{b}_i}=\sum_i{}'\overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i\mathbf{b}_i}+(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes\sum_i{}'m_i\bar{\mathbf{b}}_i.$$

It follows from the definition of $\mathbf{b}$ that the continuum form of the body-force contribution is

$$\left.\begin{aligned}&\int_R\rho(\mathbf{G}+(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{b}),\\ \text{where}\qquad&\mathbf{G}:=\lim_\varepsilon\left\{\sum_i{}'\overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i\mathbf{b}_i}\Big/m_\varepsilon\right\}.\end{aligned}\right\}\tag{4.8}$$

Particle interactions give rise to bulk and surface contributions in a now-familiar manner, the latter expressible as a sum over surface cells of terms of the form

$$\overline{\sum_i\sum_j{}'(\mathbf{x}_i-\mathbf{x}_0)\otimes\mathbf{f}_{ij}}=\overline{\sum_i\sum_j{}'(\mathbf{x}_i-\mathbf{x})\otimes\mathbf{f}_{ij}}+(\mathbf{x}-\mathbf{x}_0)\otimes\overline{\sum_i\sum_j{}'\mathbf{f}_{ij}},$$

where $\mathbf{x}$ denotes the centre of the cell in question. Use of (4.5) implies that the continuum version of the total sum is

$$\left.\begin{aligned}&\int_{\partial R}(\mathbf{C}^+ +(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{t}),\\ \text{where (cf. §3.2)}\qquad&\mathbf{C}^+:=\lim_\varepsilon\left\{\overline{\sum_i\sum_j{}'(\mathbf{x}_i-\mathbf{x})\otimes\mathbf{f}_{ij}}\Big/A_\varepsilon\right\}.\end{aligned}\right\}\tag{4.9}$$

The bulk contribution is expressible as a sum over ε-cells of terms of the form

$$\sum_i\sum_{k\neq i}{}'\overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes\mathbf{f}_{ik}},$$

each of which is independent of $\mathbf{x}_0$ *and symmetric if it is assumed* (cf. §3.1,2)

that the net time-averaged self-forces and self-couples associated with ε-cells vanish. Consequently such terms may be written as

$$\sum_{i\neq k}\sum' \overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes\mathbf{f}_{ik}},$$

giving rise to the corresponding continuum term

$$\left.\begin{aligned}&\int_R \mathbf{J},\\ &\text{where (cf. (3.28))}\\ &\mathbf{J}:=\lim_\varepsilon\left\{\sum_{i\neq k}\sum' \overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes\mathbf{f}_{ik}}\Big/V_\varepsilon\right\}\end{aligned}\right\} \tag{4.10}$$

is symmetric.

The remaining sum over particles in R involves inertial terms, the contribution to an ε-cell being

$$\sum_i' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\,d\mathbf{v}_i/dt}=d/dt\left\{\sum_i' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{v}_i}\right\}-\sum_i' \overline{\mathbf{v}_i\otimes m_i\mathbf{v}_i} \tag{4.11}$$

on using (4.3).

For solids repeated use of (4.4) together with S.1., S.3., (4.6), $(4.7)_2$ and the fluctuation-free natures of $\mathbf{x}_\varepsilon$ and $\mathbf{v}_\varepsilon$ imply that

$$\sum_i' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{v}_i}=\tilde{\mathbf{I}}\mathbf{L}^T+(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes m_\varepsilon\mathbf{v}_\varepsilon,$$

$\tilde{\mathbf{I}}$ being given by (3.11) with $\mathbf{x}_i$ replaced by $\bar{\mathbf{x}}_i$. Both $\tilde{\mathbf{I}}$ and $\dot{\tilde{\mathbf{I}}}$ are clearly of order $m_\varepsilon.O(\varepsilon^2)$, whence neglect of such terms and the assumption that $\mathbf{L}$ and $\dot{\mathbf{L}}$ are of order $O(1)$ yields

$$d/dt\left\{\sum_i' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{v}_i}\right\}=d/dt\left\{(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes m_\varepsilon\mathbf{v}_\varepsilon\right\}. \tag{4.12}$$

Further, S.1., S.3., (4.4), (4.6) and $(4.7)_2$ enable us to write (noting $\bar{\mathbf{x}}_\varepsilon=\mathbf{x}_\varepsilon$, $\bar{\mathbf{v}}_\varepsilon=\mathbf{v}_\varepsilon$)

$$\left.\begin{aligned}&\sum_i' \mathbf{v}_i\otimes m_i\mathbf{v}_i=\sum_i' \overline{\hat{\mathbf{v}}_i\otimes m\hat{\mathbf{v}}_i}+\mathbf{v}_\varepsilon\otimes m_\varepsilon\mathbf{v}_\varepsilon+\mathbf{L}\left(\tilde{\mathbf{I}}-\sum_i' \overline{\mathbf{x}_i'\otimes m_i\mathbf{x}_i'}\right)\mathbf{L}^T,\\ &\text{where}\\ &\hat{\mathbf{v}}_i:=\mathbf{v}_i-\mathbf{v}_\varepsilon-\mathbf{L}(\mathbf{x}_i-\mathbf{x}_\varepsilon).\end{aligned}\right\} \tag{4.13}$$

In the case of fluids, F.1. and F.2. imply

$$\left.\begin{aligned}&\sum_i' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\mathbf{v}_i}=(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes m_\varepsilon\mathbf{v}_\varepsilon,\\ &\text{while F.1. yields}\\ &\sum_i' \overline{\mathbf{v}_i\otimes m_i\mathbf{v}_i}=\sum_i \overline{\hat{\mathbf{v}}_i\otimes m_i\hat{\mathbf{v}}_i}+\mathbf{v}_\varepsilon\otimes m_\varepsilon\mathbf{v}_\varepsilon-\mathbf{L}\bar{\mathbf{I}}\mathbf{L}^T\end{aligned}\right\} \tag{4.14}$$

with $\mathbf{I}$ given by (3.11).

Consistent with the approximation involved in writing (4.12) is neglect of the last term in each of $(4.13)_1$ and $(4.14)_2$, and we may infer from (4.11), (4.12), $(4.13)_1$, and $(4.14)_{1,2}$ that for both solids and fluids upon neglect of terms of order $O(\varepsilon^2)$,

$$\sum_i{}' \overline{(\mathbf{x}_i-\mathbf{x}_0)\otimes m_i\, d\mathbf{v}_i/dt} = d/dt\,\{(\mathbf{x}_\varepsilon-\mathbf{x}_0)\otimes m_\varepsilon \mathbf{v}_\varepsilon\} - \sum_i{}' \overline{\hat{\mathbf{v}}_i\otimes m_i\hat{\mathbf{v}}_i} - \mathbf{v}_\varepsilon\otimes m_\varepsilon\mathbf{v}_\varepsilon.$$

Hence the continuum form for the total sum over R is

$$d/dt\left\{\int_{R_t}(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{v}\right\} - \int_R \rho(\mathbf{K}+\mathbf{v}\otimes\mathbf{v}),$$

where (4.15)

$$\mathbf{K} := \lim_\varepsilon\left\{\sum_i{}' \overline{\hat{\mathbf{v}}_i\otimes m_i\hat{\mathbf{v}}_i}\Big/ m_\varepsilon\right\}.$$

The continuum expression for generalised moment of momentum balance is, from $(4.8)_1$, $(4.9)_1$, $(4.10)_1$ and $(4.15)_1$,

$$\int_{\partial R}(\mathbf{C}^+ + (\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{t}) + \int_R (\mathbf{J}+\rho(\mathbf{G}+(\mathbf{x}-\mathbf{x}_0)\otimes\mathbf{b})) = d/dt\left\{\int_{R_t}(\mathbf{x}-\mathbf{x}_0)\otimes\rho\mathbf{v}\right\} - \int_R \rho(\mathbf{K}+\mathbf{v}\otimes\mathbf{v}). \quad (4.16)$$

The parameter $\hat{\mathbf{v}}_i$ introduced in $(4.13)_2$ and employed in the definition of $\mathbf{K}$ is clearly, to within an error of order $O(\varepsilon^2)$, the velocity of P_i relative to the bulk velocity associated with its instantaneous location. In kinetic theory (cf., e.g., Wang (**5**)) this is termed the *peculiar* velocity of P_i. It is subject to fluctuation and for a solid reduces, by $(4.7)_2$ and S.1., to

$$\hat{\mathbf{v}}_i = \mathbf{v}_i' - \mathbf{L}\mathbf{x}_i', \quad \text{so that} \quad \bar{\hat{\mathbf{v}}}_i = \mathbf{0}.$$

Working in terms of $\hat{\mathbf{v}}_i$ admits a unified treatment of solid and fluid phases, clear comparisons with kinetic theory, and simple analysis of frame-dependence of parameters.

4.3. *Energy balance*

To obtain the continuum form of energy balance for R the equations of motion of particles therein are scalarly multiplied by the corresponding velocities, summed, and then averaged over a Δ-time interval, yielding

$$\sum_i\sum_{l\neq i}\overline{\mathbf{f}_{il}\cdot\mathbf{v}_i} + \sum_i m_i\overline{\mathbf{b}_i\cdot\mathbf{v}_i} = \sum_i m_i\overline{(d\mathbf{v}_i/dt)\cdot\mathbf{v}_i}. \quad (4.17)$$

The ε-cell contribution to the body-force term is given by

$$\sum_i{}' m_i\overline{\mathbf{b}_i\cdot\mathbf{v}_i} = \sum_i{}' m_i\overline{\mathbf{b}_i\cdot\hat{\mathbf{v}}_i} + \left(\sum_i{}'\overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes m_i\mathbf{b}_i}\right).\mathbf{L}^T + \sum_i{}' m_i\bar{\mathbf{b}}_i\cdot\mathbf{v}_\varepsilon$$

which yields for the total sum the continuous form

$$\int_R \rho(\mathbf{b}.\mathbf{v}+\mathbf{G}.\mathbf{L}^T+r),$$

where (4.18)

$$r:=\lim_\varepsilon \left\{\sum_i{}' m_i\overline{\mathbf{b}_i.\hat{\mathbf{v}}_i}\Big/m_\varepsilon\right\}.$$

(Here and subsequently it is to be noted that for any vectors $\mathbf{u}$ and $\mathbf{v}$, and linear transformation $\mathbf{A}$,

$$\mathbf{u}.\mathbf{A}\mathbf{v}=\mathrm{tr}\,(\mathbf{u}\otimes\mathbf{A}\mathbf{v})=\mathrm{tr}\,((\mathbf{u}\otimes\mathbf{v})\mathbf{A}^T)=(\mathbf{u}\otimes\mathbf{v}).\mathbf{A}=(\mathbf{v}\otimes\mathbf{u}).\mathbf{A}^T,$$

tr denoting the trace operation.)

The surface contribution to the interaction sum in (4.17), namely $\overline{\sum_i\sum_j \mathbf{f}_{ij}.\mathbf{v}_i}$, yields, *in similar fashion*,

$$\left.\begin{aligned}&\int_{\partial R}(\mathbf{t}.\mathbf{v}+\mathbf{C}^+.\mathbf{L}^T+q),\\ \text{where}\quad &q:=\lim_\varepsilon\left\{\sum_i\sum_j{}'\overline{\mathbf{f}_{ij}.\hat{\mathbf{v}}_i}\Big/A_\varepsilon\right\}.\end{aligned}\right\} \tag{4.19}$$

The bulk contribution to the interaction sum in (4.17) can be argued, exactly as in section 3, to be the negative of the time derivative of the binding energy associated with R, expressible in continuum format as

$$-\frac{d}{dt}\int_R \rho w. \tag{4.20}$$

A more general alternative is obtained by noting that any ε-cell contribution may be expressed as

$$\sum_{i\neq k}\sum{}'\overline{\mathbf{f}_{ik}.\mathbf{v}_i}=\sum_{i\neq k}\sum{}'\overline{\mathbf{f}_{ik}.\hat{\mathbf{v}}_i}+\left(\sum_{i\neq k}\sum{}'\overline{(\mathbf{x}_i-\mathbf{x}_\varepsilon)\otimes\mathbf{f}_{ik}}\right).\mathbf{L}^T$$

on using the assumed vanishing of the time-averaged self-force for such cells. The foregoing yields the continuum representation

$$\left.\begin{aligned}&\int_R(\mathbf{J}.\mathbf{L}^T+P),\\ \text{where}\quad &P:=\lim_\varepsilon\left\{\sum_{i\neq k}\sum{}'\overline{\mathbf{f}_{ik}.\hat{\mathbf{v}}_i}\Big/V_\varepsilon\right\}.\end{aligned}\right\} \tag{4.21}$$

Finally, the ε-cell contribution of the right-hand side of (4.17) is, on using (4.3),

$$\sum_i{}' m_i\,\overline{d\mathbf{v}_i/dt.\mathbf{v}_i}=d/dt\left\{\sum_i{}'\tfrac{1}{2}m_i\overline{\mathbf{v}_i^2}\right\}.$$

Taking the trace of relations $(4.13)_1$ and $(4.14)_2$ and neglecting terms of order $O(\varepsilon^2)$ implies this reduces for both fluids and solids to

$$d/dt\left\{\tfrac{1}{2}\sum_i{}' m_i\overline{\hat{\mathbf{v}}_i^2}+\tfrac{1}{2}m_\varepsilon\overline{\mathbf{v}_\varepsilon^2}\right\}.$$

The continuum version for the total sum is thus

$$d/dt\left\{\int_{R_t}\rho(h+\mathbf{v}^2/2)\right\}, \tag{4.22}$$

where the (specific) *heat content* h is defined by

$$h:=\lim_\varepsilon\left\{\tfrac{1}{2}\sum_i{}' m_i\overline{\hat{\mathbf{v}}_i^2}\right\}. \tag{4.23}$$

It follows from $(4.18)_1$, $(4.19)_1$, (4.20), $(4.21)_1$, and (4.22) that the energy balance takes the form

$$\int_{\partial R}(\mathbf{t}.\mathbf{v}+\mathbf{C}^+.\mathbf{L}^T+q)+\int_R\rho(\mathbf{b}.\mathbf{v}+\mathbf{G}.\mathbf{L}^T+r)$$
$$=\int_R a+d/dt\left\{\int_{R_t}\rho(h+\mathbf{v}^2/2)\right\}, \tag{4.24}$$

where

$$a=\rho\dot{w}\quad\text{or}\quad -(P+\mathbf{J}.\mathbf{L}^T)$$

according to the viewpoint adopted on the power expended by internal interactions.

Comparison of (4.24) with the usual energy balance (cf. (**12**), equation (243.7)) leads us to identify r and q with the rates at which energy enters R by radiation from the external world and heat conduction respectively, and $(\dot{h}+a/\rho)$ with the material time derivative of the (specific) internal energy. The parameter ρh must be regarded as a measure of heat content since it is the kinetic energy density associated with thermal motion. The foregoing interpretation of r implies from $(4.18)_2$ that fluctuations in the external forces experienced by individual particles are to be identified with the effect thereon of radiation, rather than fluctuations in a body-force *field* (gravitation say). In this connection we remark that if

$$\mathbf{b}_i=\mathbf{b}(\mathbf{x}_i)+\mathbf{b}_i',$$

$\mathbf{b}_i'$ is of order $O(\varepsilon)$, and $\mathbf{b}$ is a class-C^2 field, then $\mathbf{G}$ as defined by $(4.8)_2$ is of order $O(\varepsilon^2)$ and hence negligible within our level of approximation.

4.4. *Frame-indifference*

Müller (**2**), Edelen and McLennan (**3**), and Woods (**4**) have cast doubts upon the 'principle of material frame-indifference' by citing frame-

dependent constitutive relations (for stress and heat flux) which are motivated from statistical considerations. However, it has been argued by Wang (**5**) and Speziale (**6**) that the forms of such relations depend upon approximative procedures utilised in their derivation and that it is solely these which introduce frame dependence. In what follows we show clearly the frame-indifference of the values of $\mathbf{t}$, $\mathbf{C}^+$, $\mathbf{J}$, $\mathbf{K}$, q, P, $\mathbf{J}.\mathbf{L}^T$, a, h and r provided observers agree upon which quantities are subject to fluctuation.

Recalling remark 3.4.3, specifically the assumption that *individual interactions are frame-indifferent*, and assuming that $\mathbf{c}$ *and* $\mathbf{Q}$ *are fluctuation-free*† (so that $\mathbf{c}=\bar{\mathbf{c}}, \dot{\mathbf{c}}=\hat{\mathbf{c}}=\check{\mathbf{c}}$ etc.) then from (4.5) it follows that $\mathbf{t}$ is frame-indifferent. Further, noting that in a frame change (3.33)

$$(\mathbf{x}_i-\mathbf{x}_e)\to\mathbf{Q}(\mathbf{x}_i-\mathbf{x}_e),\qquad (\mathbf{v}_i-\mathbf{v}_e)\to\mathbf{Q}(\mathbf{v}_i-\mathbf{v}_e)+\dot{\mathbf{Q}}(\mathbf{x}_i-\mathbf{x}_e),$$

$$\mathbf{L}\to\mathbf{Q}\mathbf{L}\mathbf{Q}^T+\dot{\mathbf{Q}}\mathbf{Q}^T,\qquad \hat{\mathbf{v}}_i\to\mathbf{Q}\hat{\mathbf{v}}_i,\quad\text{and}\quad \mathbf{f}_{il}\to\mathbf{Q}\mathbf{f}_{il},$$

it follows immediately from $(4.9)_2$, $(4.10)_2$, $(4.15)_2$, $(4.19)_2$, $(4.21)_2$, and (4.23) that $\mathbf{C}^+$, $\mathbf{J}$, $\mathbf{K}$, q, P and h are frame-indifferent. The symmetry and frame-indifference of $\mathbf{J}$ and the skew nature of $\dot{\mathbf{Q}}\mathbf{Q}^T$ imply $\mathbf{J}.\mathbf{L}^T$ is frame-indifferent whence the same property for w and P implies this is shared by either expression for a. Much less obviously r is frame-indifferent. To prove this it is necessary to observe that

$$\mathbf{b}_i\to\mathbf{Q}\mathbf{b}_i+\ddot{\mathbf{c}}+\ddot{\mathbf{Q}}(\mathbf{x}_i-\mathbf{x}_0)+2\dot{\mathbf{Q}}\mathbf{v}_i.$$

For solids the result follows from the fluctuational nature of $\hat{\mathbf{v}}_i$, (4.4), S.3., and the skew nature of $\dot{\mathbf{Q}}\mathbf{Q}^T$. For fluids it may be shown on using F.1., the skew nature of $\dot{\mathbf{Q}}\mathbf{Q}^T$, and noting $\sum_i{}'(\mathbf{x}_i-\mathbf{x}_e)\otimes m_i(\mathbf{x}_i-\mathbf{x}_e)/m_e$ is of order $O(\varepsilon^2)$, that

$$r\to r-\ddot{\mathbf{Q}}^T\mathbf{Q}.\mathbf{A}\mathbf{L}^T,$$

where $\mathbf{A}$ is of order $O(\varepsilon^2)$. Hence, provided $\ddot{\mathbf{Q}}^T\mathbf{Q}\mathbf{L}$ is $O(1)$, r is frame-indifferent within the approximation scheme utilised throughout this section.

Finally it is to be noted that invariance of the energy balance under superposed rigid motions is guaranteed by the analysis of 3.4.4, upon taking time averages.

5. Concluding remarks

5.1. The methodology of section 4 may be generalised to take account of large molecules. Specifically, adopting a model in which the constituent particles of individual molecules deform homogeneously and neighbouring

† In such case any set of particles having zero heat content (that is, all particles therein are fluctuation-free) with respect to one observer will share this property with all observers. Of course such observers will accordingly agree upon zero absolute temperature and vice versa. More generally, equivalent to this assumption is agreement between all observers on whether or not a given quantity is subject to fluctuation.

molecules deform in much the same way, it is possible to motivate balance relations for an unconstrained Cosserat continuum (cf. (**1**), p. 397). This approach is related to the corpuscular considerations of Dahler and Scriven (**18**), Green and Rivlin (**16**), Rivlin (**8, 19, 20**), Eringen (**8**), Eringen and Suhubi (**21, 22**), Capriz and Podio Guidugli (**23, 24**), and Alblas (**14**). However, with the exception of Dahler and Scriven and of Alblas, whose viewpoint was that of statistical mechanics, these authors did not consider thermal motions, and none emphasised the necessity of similar deformations for near-neighbours. A special case of the foregoing models materials composed of very long molecules which, in some phase, tend to align with each other (for example, materials with a liquid crystalline phase). Here the work amplifies and complements the pioneering contributions of Ericksen (**25, 26**) in respect of the theory of liquid crystals.

5.2. The particle viewpoint readily motivates the kinematics of mixtures and has implications, for example, in respect of partial stresses and heat fluxes.

5.3. If intermolecular forces have significant long-range effects (that is, have ranges well in excess of 1000 Å) our discussion might suggest the concept of stress to be meaningless. However, interactions are composites of forces of differing character: those of short-range may be considered as furnishing an appropriate δ as in section 3, hence yielding a stress field which takes account of the *total* interaction up to this cut-off. The remainder of the interaction is non-local and must, of course, include gravitation. Since the latter is well-understood, it would appear that non-local theories address interactions of an electromagnetic nature which differ from those normally considered (cf. (**11**) and Moelwyn-Hughes (**27**)). Indeed, as remarked in the Introduction, interactions are described as of very long range if $\delta \sim 200$ Å (cf. (**11**)), while in this work it has been shown that even with $\delta \sim 1000$ Å strictly local *continuum* theories result.

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