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Balance equations for physical systems with corpuscular structure

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Abstract

The usual method in nonequilibrium statistical mechanics allows the derivation of the balance equations only for the collision invariants (mass, momentum, energy) and only by a complete knowledge of the microscopic structure. In this paper the existence of the balance equation for an arbitrary physical quantity is proved for any corpuscular system satisfying the local equilibrium assumption, if the microscopic components obey the classical mechanics principles and can be generated or destroyed as a result of some instantaneous processes. We discuss the fundamental equations of the continuum mechanics for mass and momentum.

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1. Introduction

The balance equations are postulated relations for fundamental physical quantities (mass, momentum, energy, entropy, etc.) valid for all continuous media [1]. We take over the differential expression of the balance equations from Ref. [2]. Let Ψ be an additive physical quantity associated to a continuous medium. That is, there exists a function Ψ of space ($\boldsymbol{r}$) and time (t), called the volume density of Ψ, such that, for any volume V, the integral $\int_V \Psi \, \mathrm{d}\boldsymbol{r}$ represents the amount of Ψ contained in V. The differential form of the balance equation at a regular point (i.e. without shocks or other discontinuities) is

$$\partial_t \Psi + \sum_{\alpha=1}^{3} \partial_\alpha (\Phi_\alpha + \Psi V_\alpha) - (p + s) = 0, \tag{1}$$

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where ∂_t is the temporal derivative, ∂_α is the derivative with respect to the α component of $\boldsymbol{r}$, Φ_α is the α component of the flux density of Ψ, v_α is the α component of the velocity, p is the production density of Ψ due to interior processes and s is the supply density of Ψ controlled from the exterior of V. The quantities $\boldsymbol{\Phi}$, p and s are expressed by the constitutive equations characterizing the considered material.

The statistical method of derivation of the balance equations for a macroscopic physical system from its microscopic structure was initiated by Boltzmann [3–5]. We shall consider only the classical nonequilibrium statistical mechanics. This method relies on the evolution equation of the probability density in the phase space for the system consisting of all the microscopic components of the physical system (Liouville equation). Even for the simple case of the ideal gas, because of mathematical difficulties, the derivation of the balance equations and constitutive equations is possible only using certain hypotheses, approximations and simplifications [6]. So far, these results have been extended to hard sphere fluids, also a very idealized molecular model [7]. For a more complicated microscopic structure, the existence of the balance equations is implicitly *postulated* and the problem of the statistical mechanics is reduced to the calculation of the constitutive equations.

In this paper we show that the balance equations can be derived in three successive stages. First we prove that for an arbitrary finite number of material points, a space–time average satisfying a mathematical relation of the form (1) can be defined. The corpuscular structure of a physical system ensures the existence of mathematical relations of the balance equations even if the space–time averages have discontinuous first order partial derivatives. In the second stage we obtain the smoothness specific to the continuous fields if the physical system verifies the local equilibrium assumption. Thus, balance equation (1) follows only from two hypotheses: the corpuscular structure and the local equilibrium assumption. In the third stage, the information on the microscopic structure is used to derive the constitutive equations.

The usual statistical approach does not allow the separation of these three stages, all of them being simultaneously implied in the Liouville equation. The mathematical form specific to balance equations is implicitly contained in the Liouville equation which is a probability conservation law in phase space. The smoothness characteristic to continuous fields is introduced by the probability density in phase space which is defined as a continuous field. The Liouville equation can be written only if the interaction forces of the microscopic components are known, i.e. the model of the microscopic structure of the physical system has to be completely described.

A finite number of particles satisfying the classical mechanics principles is the physical system with corpuscular structure considered in the following. The particles are modelled as material points, i.e. all the physical quantities necessary to describe the structure of the particles are assigned to mathematical points defining the position of the particles. The particles can appear or disappear as a result of some instantaneous processes (e.g. chemical reactions). We assume that the evolution of any physical quantity chacterizing the particles is given by an analytic function of time. Under these circumstances we shall prove that a space–time average of an arbitrary

physical quantity has a.e. continuous partial derivatives. Although these averages preserve the discontinuities associated to the particles as discontinuity surfaces, they satisfy a relation of the form (1). In the following, such a relation will be called "the discrete analogue" of a similar relation in continuum mechanics.

At the end, the balance equation for an arbitrary physical quantity is obtained using the local equilibrium assumption. As an example, we prove the existence of the balance equations for mass and momentum. These equations have the same form as in continuum mechanics if the following hypotheses on the microscopic structure are used: there is a single type of microscopic components and the interaction of the particles has a spherical symmetry. The general problem of the derivation of the constitutive equations from the microscopic structure is briefly discussed. It will be the subject of future articles on physical systems with complex microscopic structure.

2. The discrete analogue of continuous fields

We study the evolution during the temporal interval $I = [0, T] \subset \mathbb{R}$ of a discrete system consisting on N particles obeying the principles of classical mechanics. We denote by $I_i = [t_i^+, t_i^-] \subset I$ the existence interval of the ith particle ($1 \leqslant i \leqslant N$). Let $n(t)$ be the number of the particles existing at the moment $t \in I$. The variations of $n(t)$ occur when some particles are generated or destroyed. It is obvious that $n(t) \leqslant N$ for each $t \in I$, and $n(t) = N$ for all $t \in I$ only if $I_i = I$ for each $i \leqslant N$, i.e. if no particles are generated or destroyed over the interval I.

Let φ be an arbitrary physical quantity. The values of φ characterizing the ith particle are given by a function $\varphi_i: I \to \mathbb{R}$. If $I_i \neq I$, then $\varphi_i(t) = 0$ for all $t \in I \setminus I_i$. We assume that the restriction $\varphi_i | I_i$ can be represented as a Taylor series, i.e., it is an analytic function. In the interval I_i the quantity φ_i may take any real value, including zero (e.g., the velocity components of a motionless particle). Hence φ_i is discontinuous at t_i^+ and t_i^- if $\varphi_i(t_i^+) \neq 0$ and $\varphi_i(t_i^-) \neq 0$, respectively. Similarly, the derivatives of φ_i at t_i^+ and t_i^- may be continuous or discontinuous.

We assign to each particle a mathematical point indicating its position. The choice of the particle mass center is always possible; other options may be also adopted under the restriction that the mathematical point should be uniquely defined. To these mathematical points we assign the microscopic quantities φ_i describing the evolution of the particles. The number and the type of these quantities depend on the properties and the complexity of the particles. Thus the discrete system is modelled as a finite set of material points. The α components of the radius vector $\boldsymbol{r}_i$, $x_{\alpha i}: I \to \mathbb{R}$ ($\alpha = 1, 2, 3$), and of the velocity $\boldsymbol{\xi}_i$, $\xi_{\alpha i}: I \to \mathbb{R}$ ($\alpha = 1, 2, 3$) may be treated as particular cases of functions φ_i. The functions $x_{\alpha i}$ and $\xi_{\alpha i}$ supply a kinematic description of the motion of the discrete system. The assumption that each particle obeys the principles of classical mechanics is necessary to ensure the uniqueness of the discrete system evolution and thus, the existence of the functions φ_i. The moments when the solutions of Hamilton's equations are not analytic may be considered moments when new particles are

generated. For example, an instantaneous perfectly elastic collision does not change the type of the particles, but the velocity discontinuity may be associated with the generation of new particles of the same type as the old ones with different velocities. We assume that the instantaneous discontinuous processes are of finite number over the interval $I = [0, T]$.

We intend to characterize the mean distribution of φ about the point of radius vector $\boldsymbol{r}$ at the moment t. Therefore we average the values φ_i corresponding to the particles lying in the open sphere of center $\boldsymbol{r}$ and radius a denoted $S(\boldsymbol{r}, a)$, over the interval $(t-\tau, t+\tau)$. Here $\tau < T$ and a are arbitrary positive real parameters. We define the mean distribution of φ as a function D_φ: $\mathbb{R}^3 \times (\tau, T-\tau) \to \mathbb{R}$ with

$$D_\varphi(\boldsymbol{r}, t) = \frac{1}{2\tau V} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} \varphi_i(t') H^+(a^2 - (\boldsymbol{r}_i(t') - \boldsymbol{r})^2)\, \mathrm{d}t', \tag{2}$$

where $V = 4\pi a^3/3$ is the volume of $S(\boldsymbol{r}, a)$ and H^+ is the left continuous Heaviside function. Since $H^+(a^2 - (\boldsymbol{r}_i(t') - \boldsymbol{r})^2)$ vanishes if the ith particle is located outside the sphere $S(\boldsymbol{r}, a)$ and $\varphi_i(t')$ vanishes if $t' \in I \setminus I_i$, then a nonvanishing contribution to D_φ is due only to particles which lie in $S(\boldsymbol{r}, a)$ over the interval $(t-\tau, t+\tau)$.

The function $H^+(a^2 - (\boldsymbol{r}_i(t) - \boldsymbol{r})^2)$ in (2) takes only the values 0 and 1. The jumps occur when the ith particle enters or leaves the open sphere $S(\boldsymbol{r}, a)$. These moments are among the solutions u_i of the equation

$$h_i(\boldsymbol{r}, u_i) \equiv (\boldsymbol{r}_i(u_i) - \boldsymbol{r})^2 - a^2 = 0, \tag{3}$$

where $|h_i(\boldsymbol{r}, t)|^{1/2}$ is the distance at the moment t between the ith particle and the surface $\partial S(\boldsymbol{r}, a)$ of the sphere $S(\boldsymbol{r}, a)$. Since $x_{\alpha i}$, and hence h_i, are analytic functions with respect to u_i, and I_i is closed interval, then either Eq. (3) has a finite number of solutions or h_i vanishes identically [8].

In the latter case the particle moves along the surface of $S(\boldsymbol{r}, a)$ and does not enter the sphere, hence $H^+(a^2 - (\boldsymbol{r}_i(t) - \boldsymbol{r})^2)$ is identically zero and has no jumps. Since $\boldsymbol{r}_i(u_i)$ is a known function, then the isolated zeros of (3) are implicit functions $u_i(\boldsymbol{r})$. The implicit function theorem can be applied only at interior points and it does not ensure the existence of $u_i(\boldsymbol{r})$ for $u_i = t_i^{\pm}$, i.e. $\boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t_i^{\pm}), a)$. This case will be discussed separately. For $u_i \in (t_i^+, t_i^-)$, if

$$\partial h_i / \partial u_i = 2(\boldsymbol{r}_i(u_i) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u_i) \neq 0, \tag{4}$$

then the function $u_i(\boldsymbol{r})$ exists in a neighborhood of $\boldsymbol{r}$ and has the derivatives

$$\frac{\partial u_i}{\partial x_\alpha} = -\frac{\partial h_i}{\partial x_\alpha} \Big/ \frac{\partial h_i}{\partial u_i} = \frac{x_{\alpha i}(u_i) - x_\alpha}{(\boldsymbol{r}_i(u_i) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u_i)}, \qquad \alpha = 1, 2, 3, \tag{5}$$

where x_α are the components of $\boldsymbol{r}$. According to (4), the function $u_i(\boldsymbol{r})$ is not differentiable at the points of the discriminant surface of the family $\{\partial S(\boldsymbol{r}_i(t), a);\ t \in I_i\}$.

We denote the moments when the ith particle enters (leaves) the sphere $S(\boldsymbol{r}, a)$ by $t_i^+ < u'_{i1} < u'_{i2} < \cdots < u'_{in'} < t_i^-$ ($t_i^+ < u''_{i1} < u_{i2} < \cdots < u''_{in''} < t_i^-$). Since the sphere $S(\boldsymbol{r}, a)$ is open, $H^+(a^2 - (\boldsymbol{r}_i(t) - \boldsymbol{r})^2)$ as a function of t is left (right) continuous when the particle enters (leaves). Hence for $t \in I_i$, we have

$$H^+(a^2 - (\boldsymbol{r}_i(t) - \boldsymbol{r})^2) = H^+(a^2 - (\boldsymbol{r}_i(t_i^+) - \boldsymbol{r})^2) + \sum_{k'=1}^{n'} H^+(t - u'_{ik'}) - \sum_{k''=1}^{n''} H^-(t - u''_{ik''}), \tag{6}$$

where H^- is the right continuous Heaviside jump function. The first term in the right-hand side of (6) vanishes if the ith particle is generated in the exterior of $S(\boldsymbol{r}, a)$ and equals 1 otherwise. If $u_i = t_i^+$, then the particle can only enter the sphere after its generation, hence $u'_{i1} = t_i^+$ and relation (6) holds. If $u_i = t_i^-$, then the particle could only leave the sphere before its disappearance, hence $u''_{in''} = t_i^-$ and relation (6) holds again. So (6) contains all the possible situations if we take $t_i^+ \leqslant u'_{i1}$ and $u''_{in''} \leqslant t_i^-$. The following notation will be used:

$$U'_i = \{u'_{i1}, u'_{i2}, \ldots, u'_{in'}\}, \qquad U''_i = \{u''_{i1}, u''_{i2}, \ldots, u''_{in''}\}. \tag{7}$$

To study the differentiability of D_φ, we consider the function g_i: $\mathbb{R}^3 \times (\tau, T - \tau) \to \mathbb{R}$

$$g_i(\boldsymbol{r}, t) = \int_{t-\tau}^{t+\tau} \varphi_i(t') H^+(a^2 - (\boldsymbol{r}_i(t') - \boldsymbol{r})^2)\, dt'. \tag{8}$$

For a fixed $\boldsymbol{r}$, the integrand

$$G_i(\boldsymbol{r}, t) = \varphi_i(t) H^+(a^2 - (\boldsymbol{r}_i(t) - \boldsymbol{r})^2) \tag{9}$$

is a continuous function, except a finite number of jump discontinuities $\{t_i^+, t_i^-\} \cup U'_i \cup U''_i$. Hence G_i is Riemann integrable and g_i has partial derivative with respect to t a.e. in $(\tau, T - \tau)$, equal to

$$\partial_t g_i(\boldsymbol{r}, t) = G_i(\boldsymbol{r}, t + \tau) - G_i(\boldsymbol{r}, t - \tau). \tag{10}$$

The discontinuities of $\partial_t g_i$ with respect to $(\boldsymbol{r}, t)$ are related to those of G_i. From (9) it follows that G_i is discontinuous when φ_i is discontinuous and H^+ nonvanishing, or conversely, when H^+ is discontinuous and φ_i nonvanishing. In the first case the ith particle appears or disappears in $S(\boldsymbol{r}, a)$, i.e. $t = t_i^\pm$ and $\boldsymbol{r} \in S(\boldsymbol{r}_i(t_i^\pm), a)$, and in the second case the ith particle lies in the surface of $S(\boldsymbol{r}, a)$, i.e. $t \in I_i$ and $\boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t), a)$. Hence the derivative (10) is not continuous over

$$\Omega'_i = \{(\boldsymbol{r}, t) \mid t \in \{t_i^\pm - \tau, t_i^\pm + \tau\} \cap (\tau, T - \tau) \text{ and } \boldsymbol{r} \in S(\boldsymbol{r}_i(t_i^\pm), a)\} \cup \{(\boldsymbol{r}, t) \mid t \in [t_i^+ \pm \tau, t_i^- \pm \tau] \cap (\tau, T - \tau) \text{ and } \boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t \mp \tau), a)\}. \tag{11}$$

The set Ω'_i has null Lebesgue measure in $\mathbb{R}^3 \times (\tau, T - \tau)$, hence $\partial_t g_i$ is a.e. continuous.

Although (6) holds only for $t \in I_i$, it may be substituted in (8) because φ_i vanishes for $t \in I \setminus I_i$. The obtained expression allows the study of the differentiability with respect to $\boldsymbol{r}$ of the function g_i. There exist three possible situations, namely: $2\tau \leqslant t_i^- - t_i^+$, $\tau < t_i^- - t_i^+ < 2\tau$ and $t_i^- - t_i^+ \leqslant \tau$. For each of them the discussion, although elementary, is rather long and involved [9]. Here we give only the result. The set where the function g_i is not differentiable with respect to $\boldsymbol{r}$ is

$$\begin{aligned}\Omega_i'' = &\{(\boldsymbol{r},t) |\, t \in (t_i^+ - \tau, t_i^+ + \tau] \cap (\tau, T-\tau) \text{ and } \boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t_i^+), a)\} \\ &\cup \{(\boldsymbol{r},t) |\, t \in [t_i^- - \tau, t_i^- + \tau) \cap (\tau, T-\tau) \text{ and } \boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t_i^-), a)\} \\ &\cup \{(\boldsymbol{r},t) |\, t \in (t_i^+ \pm \tau, t_i^- \pm \tau) \cap (\tau, T-\tau) \text{ and } \boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t \mp \tau), a)\} \\ &\cup \{(\boldsymbol{r},t) |\, t \in (\tau, T-\tau), \text{ exists } t' \in (t-\tau, t+\tau) \cap I_i \text{ such that} \\ &\quad \boldsymbol{r} \in \partial S(\boldsymbol{r}_i(t'), a) \text{ and } (\boldsymbol{r}_i(t') - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(t') = 0\},\end{aligned} \tag{12}$$

and it is of null Lebesgue measure in $\mathbb{R}^3 \times (\tau, T-\tau)$. The derivative of g_i with respect to x_α, denoted by $\partial_\alpha g_i$, is

$$\partial_\alpha g_i(\boldsymbol{r},t) = \sum_{u \in U_i} \varphi_i(u) \frac{x_{\alpha i}(u) - x_\alpha}{|(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)|}, \tag{13}$$

where $U_i = (U_i' \cup U_i'') \cap (t-\tau, t+\tau)$.

Using definition (2) and relations (10)–(13), it follows the a.e. continuity of the partial derivatives of D_φ, given by

$$\partial_t D_\varphi(\boldsymbol{r},t) = \frac{1}{2\tau V} \sum_{i=1}^{N} [G_i(\boldsymbol{r}, t+\tau) - G_i(\boldsymbol{r}, t-\tau)], \tag{14}$$

for $(\boldsymbol{r},t) \in \mathbb{R}^3 \times (\tau, T-\tau) \setminus \bigcup_{i=1}^N \Omega_i'$, and

$$\partial_\alpha D_\varphi(\boldsymbol{r},t) = \frac{1}{2\tau V} \sum_{i=1}^{N} \sum_{u \in U_i} \varphi_i(u) \frac{x_{\alpha i}(u) - x_\alpha}{|(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)|}, \tag{15}$$

for $(\boldsymbol{r},t) \in \mathbb{R}^3 \times (\tau, T-\tau) \setminus \bigcup_{i=1}^N \Omega_i''$. The a.e. continuity of the partial derivatives ensures the continuity of D_φ with respect to $(\boldsymbol{r},t) \in \mathbb{R}^3 \times (\tau, T-\tau)$ and then D_φ is a continuous field.

3. The discrete analogue of the balance equation

In the following we shall derive the relation satisfied by D_φ. We use a theorem stating that every function with bounded variation may be uniquely split into a sum of

two functions: one continuous and a jump function [10]. We apply this theorem to G_i given by (9) considered as a function of t. But except a finite number of jump discontinuities, G_i is analytic on I and then its continuous part G_i' is also absolutely continuous. Hence we may write $G_i = G_i' + G_i''$, where G_i'' is the jump function. Replacing this relation in (14), it follows that $\partial_t D_\varphi$ can also be written as a two-term sum

$$\partial_t D_\varphi = (\partial_t D_\varphi)' + (\partial_t D_\varphi)''. \tag{16}$$

According to the Lebesgue theorem, the absolutely continuous part of G_i is equal to the integral of the derivative of G_i

$$G_i'(\boldsymbol{r}, t+\tau) - G_i'(\boldsymbol{r}, t-\tau) = \int_{t-\tau}^{t+\tau} \frac{\partial G_i}{\partial t}(\boldsymbol{r}, t')\, dt'$$

$$= \int_{t-\tau}^{t+\tau} \dot{\varphi}_i(t') H^+(a^2 - (\boldsymbol{r}_i(t') - \boldsymbol{r})^2)\, dt'. \tag{17}$$

Dividing (17) by $2\tau V$, summing up with respect to i, taking into account (9), (14) and (2) we obtain the part of $\partial_t D_\varphi$ resulting from G_i',

$$(\partial_t D_\varphi)' = D_{\dot{\varphi}}. \tag{18}$$

From (14), the discontinuous part of $\partial_t D_\varphi$ can be written as

$$(\partial_t D_\varphi)''(\boldsymbol{r}, t) = \frac{1}{2\tau V} \sum_{i=1}^{N} [G_i''(\boldsymbol{r}, t+\tau) - G_i''(\boldsymbol{r}, t-\tau)] \tag{19}$$

It contains the discontinuous variations of G_i during the temporal interval $[t-\tau, t+\tau]$. As proved in the preceding section, $\partial_t D_\varphi$ exists if G_i is not discontinuous at $t+\tau$ and $t-\tau$ (see expression (11)), therefore we consider only the jumps occurring at the interior points of $[t-\tau, t+\tau]$, i.e. in $(t-\tau, t+\tau)$. From (9) it follows that such a variation can take place if the particle is generated inside the sphere $S(\boldsymbol{r}, a)$ during the temporal interval $(t-\tau, t+\tau)$. Hence the jump of G_i is equal to

$$\Delta^+ G_i = \varphi_i(t_i^+) H^+(a^2 - (\boldsymbol{r}_i(t_i^+) - \boldsymbol{r})^2)(H^+(t+\tau-t_i^+) - H^-(t-\tau-t_i^+)).$$

Similarly, the discontinuous variation of G_i related to the distruction of a particle is

$$\Delta^- G_i = -\varphi_i(t_i^-) H^+(a^2 - (\boldsymbol{r}_i(t_i^-) - \boldsymbol{r})^2)(H^+(t+\tau-t_i^-) - H^-(t-\tau-t_i^-)).$$

The function G_i also has discontinuous variations when the particle enters or leaves the sphere $S(\boldsymbol{r}, a)$,

$$G_i''(\boldsymbol{r}, t+\tau) - G_i''(\boldsymbol{r}, t-\tau) = \Delta^+ G_i + \Delta^- G_i + \sum_{u \in W_i^+} \varphi_i(u) - \sum_{u \in W_i^-} \varphi_i(u), \tag{20}$$

where $W_i' = U_i' \cap (t-\tau, t+\tau)$ and $W_i'' = U_i'' \cap (t-\tau, t+\tau)$. The sign of $\varphi_i(u)$ is positive (negative) if the particle enters (leaves) the sphere $S(\boldsymbol{r}, a)$, and it is given by the sign of the expression $-(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)$ which is proportional to the interior normal component of $\boldsymbol{\xi}_i$ to the surface of $S(\boldsymbol{r}, a)$ at the moment u. Hence we may use a single sum in (20) if we denote, as in (13), $U_i = W_i' \cup W_i''$. Replacing (20) in (19) we obtain

$$(\partial_t D_\varphi)'' = (\partial_t D_\varphi)_g - \frac{1}{2\tau V} \sum_{i=1}^{N} \sum_{u \in U_i} \varphi_i(u) \frac{(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)}{|(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)|}, \tag{21}$$

where

$$(\partial_t D_\varphi)_g = \frac{1}{2\tau V} \sum_{i=1}^{N} (\Delta^+ G_i + \Delta^- G_i). \tag{22}$$

Relation (15) for the physical quantity $\varphi_i \xi_{\alpha i}$ reads

$$\partial_\alpha D_{\varphi \xi_\alpha} = \frac{1}{2\tau V} \sum_{i=1}^{N} \sum_{u \in U_i} \varphi_i(u) \xi_{\alpha i}(u) \frac{x_{\alpha i}(u) - x_\alpha}{|(\boldsymbol{r}_i(u) - \boldsymbol{r}) \cdot \boldsymbol{\xi}_i(u)|}.$$

Comparing this relation with (21) we obtain

$$(\partial_t D_\varphi)'' = -\sum_{\alpha=1}^{3} \partial_\alpha D_{\varphi \xi_\alpha} + (\partial_t D_\varphi)_g. \tag{23}$$

From (16), (18) and (23) follows the relation

$$\partial_t D_\varphi + \sum_{\alpha=1}^{3} \partial_\alpha D_{\varphi \xi_\alpha} = D_{\dot{\varphi}} + (\partial_t D_\varphi)_g. \tag{24}$$

This relation holds only when the derivatives (14) and (15) exist.

In contrast to balance equation (1), relation (24) does not contain a quantity equivalent to the velocity $\boldsymbol{v}$. The velocity is not a volume density, but an average quantity. To define a discrete analogue, we must divide D_φ by the number of the particles contributing to D_φ. Let D_1 be the density D_φ corresponding to $\varphi_i(t) = 1$ for all $t \in I_i$ and $i \leqslant N$. Since D_1 characterizes the average number of particles per unit volume, the discrete average of φ is defined as

$$\bar{\varphi}(\boldsymbol{r}, t) = D_\varphi(\boldsymbol{r}, t) / D_1(\boldsymbol{r}, t) \tag{25}$$

if $D_1(\boldsymbol{r}, t) \neq 0$, and it vanishes if $D_1(\boldsymbol{r}, t) = 0$. It is easy to show that $\bar{\bar{\varphi}} = \bar{\varphi}$, $\overline{\varphi_1 + \varphi_2} = \overline{\varphi_1} + \overline{\varphi_2}$ and $\overline{\lambda \varphi} = \lambda \bar{\varphi}$, where λ is a real function of $\boldsymbol{r}$ and t.

The mean motion of the particles is given by the discrete average of the velocity $\bar{\boldsymbol{\xi}}$ with the components $\bar{\xi}_\alpha$. To introduce $\bar{\xi}_\alpha$ in (24), we write

$$D_{\varphi \xi_\alpha} = D_{\varphi[\bar{\xi}_\alpha + (\xi_\alpha - \bar{\xi}_\alpha)]} = \bar{\xi}_\alpha D_\varphi + (\boldsymbol{\Phi}_\varphi')_\alpha,$$

where $\boldsymbol{\Phi}_\varphi'$ is the discrete analogue of the kinetic part of the flux density

$$\boldsymbol{\Phi}_\varphi' = \sum_{\alpha=1}^{3} D_{\varphi(\xi_\alpha - \bar{\xi}_\alpha)} \boldsymbol{e}_\alpha,$$

$\boldsymbol{e}_\alpha$ being the unit vectors in ordinary three-dimensional space. Then (22) becomes

$$\partial_t D_\varphi + \nabla\cdot(D_\varphi\bar{\boldsymbol{\xi}}) + \nabla\cdot\boldsymbol{\Phi}'_\varphi = D_{\dot{\varphi}} + (\partial_t D_\varphi)_g. \tag{26}$$

This is the discrete analogue of the balance equation (1).

4. The continuous modelling

The discrete analogues of continuous fields (2) and of balance equations (26) have an intermediate status between the microscopic discrete description of a physical system and its macroscopic description by means of continuous fields, having characteristics in common with both.

As in the microscopic discrete description, we imposed no limits on the number of particles, whereas it is known that the continuous modelling is possible only for a large number of particles. Then, the complete knowledge of the function D_φ given by (2) (including the points where it is not differentiable) is equivalent to the knowledge of the evolution of the microscopic state for all the N particles. On the contrary, the macroscopic continuous fields are characterized by smearing out the discontinuities of microscopic nature.

The main similarities between our results and the macroscopic continuous description are the following. Using only microscopic physical quantities, we have constructed a physical quantity satisfying relation (26), formally identical with the macroscopic balance equation (1). Moreover, relation (26) has the same generality as its macroscopic correspondent, being valid for any physical quantity and for any physical system with corpuscular structure.

In order to obtain the balance equation (1), we have to eliminate from (26) the discontinuities specific to the microscopic scale. In statistical physics these discontinuities are eliminated from the very beginning, since the probability density in phase space has the smoothness properties of a continuous field. The usual statistical average may be applied to relation (26) and the balance equation (1) is obtained for $\tau \to 0$ and $a \to 0$. In this article we do not present this approach, but a shorter and more intuitive one, although less rigorous.

The linear thermodynamics of irreversible processes can be applied to far-from-equilibrium states if the local equilibrium assumption is satisfied [11]. Then at any time and for any point there exists a microscopic part of the macroscopic body acting as a near-equilibrium thermodynamic system. In our case we choose the parameters a and τ such that over the interval $(t - \tau, t + \tau)$ the particles in the sphere $S(\boldsymbol{r}, a)$ should form the near-equilibrium thermodynamic system. It is obvious that the space–time average (2) and the discrete average (25) become the corresponding continuous fields and the relation (26) becomes a balance equation. The local equilibrium assumption eliminates the microscopic discontinuities due to the large number of particles contributing to the value of D_φ. This condition was also used by Murdoch [12] to

smooth the microscopic discontinuities by a space–time averaging. The main difference is that in our approach the smoothing is made after a relation of the form (1) was obtained. Similarly to the usual statistical method, Murdoch obtains at the same time both the mathematical form of the balance equation and the smoothness characteristic to macroscopic continuous fields.

On the other hand, the parameters a and τ must be smaller than the spatial and temporal characteristic magnitude of the considered physical process. Otherwise the modelled process is distorted. For example, in the case of a plane wave, the wavelength and the period must be much larger than a and τ, respectively.

Thus the existence of the balance equation for any physical quantity has been proved, but its explicit form depends on the microscopic structure of the physical system. As an example, in the following we derive the fundamental equations of continuum mechanics, the balance equation for mass and momentum, in the simple case of identical particles. Otherwise the equations would become much more involved because of additional diffusive terms. Since there is only one type of particles, processes like chemical reactions are excluded. Thus the appearance or disappearance of the particles may be related only to the discontinuous variations of certain physical quantities as velocity, momentum, etc. This situation occurs, for example, if the collisions of the particles can be modelled as instantaneous processes of discontinuous variations of the momentum or if the particles interact instantaneously with exterior fields (e.g., photons in the Compton effect).

First, for each microscopic component we must uniquely define the mathematical point determining its position and the physical quantities necessary to describe its state. The relation (26) can be written for each of these physical quantities. Whatever the structure of the microscopic components, their mass and position are always uniquely defined, and hence their momentum too. Thus the balance equations for mass and momentum exist for any corpuscular physical system.

The relation (26) for mass is obtained if $\varphi_i(t) = m$ for all $t \in I_i$ and $i \leqslant N$, where m is the mass of the particles. Then $D_\varphi = D_m = mD_1$ is the discrete analogue of the mass density. Since there is only one type of particles, the appearance or disappearance of the particles does not imply mass variations, hence $(\partial_t D_m)_g = 0$. Moreover, $\bar{\varphi} = m$, $\boldsymbol{\Phi}'_m = 0$, $\dot{\varphi}_i = 0$ and (26) becomes

$$\partial_t D_m + \nabla\cdot(D_m \bar{\boldsymbol{\xi}}) = 0. \tag{27}$$

This is the discrete analogue of the continuity equation.

For the α component of momentum we have $\varphi_i = p_{\alpha i} = m\xi_{\alpha i}$ and $D_{p_\alpha} = D_{m\xi_\alpha} = D_m \bar{\xi}_\alpha$. The discrete analogue of the kinetic part of the flux density takes the form of a symmetric tensor

$$T'_{\alpha\beta} = (\boldsymbol{\Phi}'_{p_\alpha})_\beta = -\frac{m}{2\tau V} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} (\xi_{\alpha i}(t') - \bar{\xi}_\alpha)(\xi_{\beta i}(t') - \bar{\xi}_\beta) \times H^+(a^2 - (\boldsymbol{r}_i(t') - \boldsymbol{r})^2)\, dt'. \tag{28}$$

The derivative $\dot{\varphi}_i$ is the α component of the force $\boldsymbol{f}_i$ acting on the ith particle and relation (26) becomes

$$\partial_t(D_m\bar{\xi}_\alpha) + \sum_{\beta=1}^{3} \partial_\beta(D_m\bar{\xi}_\alpha\bar{\xi}_\beta) - \sum_{\beta=1}^{3} \partial_\beta T'_{\alpha\beta} = D_{f_\alpha} + (\partial_t D_{p_\alpha})_\theta \,. \tag{29}$$

This relation takes a form identical with the balance equation for momentum in continuum mechanics only if additional hypotheses on the microscopic structure are made.

As discussed above, the parameters a and τ are chosen so that the local equilibrium assumption should hold and space–time average (2) should not distort the modelled process. Then the space–time averages D_1 and D_m become the concentration $c(\boldsymbol{r}, t)$ and the mass density $\rho(\boldsymbol{r}, t)$, respectively, which are continuous fields and the discrete average of the velocity $\bar{\boldsymbol{\xi}}$ becomes the continuous field of velocity $\boldsymbol{v}(\boldsymbol{r}, t)$. Then from relation (27) we obtain the continuity equation

$$\partial_t\rho + \nabla\cdot(\rho\boldsymbol{v}) = 0 \,. \tag{30}$$

The symmetric tensor (28) becomes the kinetic contribution to stress tensor $\sigma'_{\alpha\beta}$ [13]. The force term in (29) is the sum of the contributions due to the external potential $U(\boldsymbol{r}, t)$ and interaction forces between the particles. Since the values of a and τ were chosen so that the variation of U in the sphere $S(\boldsymbol{r}, a)$ over the interval $(t - \tau, t + \tau)$ should be negligible, the first contribution equals $-c\nabla U$. Then relation (29) becomes

$$\partial_t(\rho v_\alpha) + \sum_{\beta=1}^{3} \partial_\beta(\rho\boldsymbol{v}_\alpha\boldsymbol{v}_\beta) - \sum_{\beta=1}^{3} \partial_\beta\sigma'_{\alpha\beta} - cF_\alpha = -c\partial_\alpha U + P_\alpha \,, \tag{31}$$

where $\boldsymbol{F}(\boldsymbol{r}, t)$ is the continuous field representing the mean force acting at the moment t on a particle placed at $\boldsymbol{r}$ due to the interaction with the other particles, and $\boldsymbol{P}(\boldsymbol{r}, t)$ is the momentum production at the time t and the point $\boldsymbol{r}$.

The number of the continuous fields in the balance equations (30) and (31) can be decreased if further hypotheses on the microscopic structure are introduced. For example, if the interaction potential is a continuous function, then the momentum variations of the particles are continuous and $\boldsymbol{P} = 0$. If, in addition, the interparticle forces have spherical symmetry, then the term $c\boldsymbol{F}$ in (31) is the divergence of a symmetric tensor [13] and (31) becomes the usual momentum balance equation of continuum mechanics.

5. Conclusion

The existence of balance equations has been proved for corpuscular physical systems satisfying the local equilibrium assumption. We have obtained this result under circumstances similar to the most general ones in continuum mechanics: the microscopic components can be generated or destroyed as a result of some instantaneous processes (chemical reactions, collisions, etc.) and the balance equation is derived for an arbitrary physical quantity.

As in kinetic theory, we have assumed that the microscopic components obey the classical mechanics principles, but in kinetic theory the balance equations are derived under more restrictive conditions [3–5]. The derivation of the Boltzmann equation from the Liouville equation requires a series of assumptions: the molecular chaos hypothesis, biparticle collisions, central interaction forces, etc. Besides, the balance equations can be obtained only for the collision invariants (mass, momentum, energy). We avoided these limitations since not all the information on the microscopic structure was introduced from the very beginning. In the first stage we have showed that for a finite number of material points the space–time average (2) satisfies a mathematical relation of the same form as the balance equations. In the second stage we have used the local equilibrium assumption which ensures the necessary smoothness for the continuous fields. Only in the last stage the particular microscopic structure of the physical system has been taken into account. In this article the microscopic structure has been specified only as far as to obtain the fundamental momentum balance equation of the continuum mechanics, i.e. we have considered only one type of particles with spherical symmetry.

The method exposed above may present a supplementary interest in the case of a complex microscopic structure. The more complex the microscopic structure, the more numerous are the simplifications and approximations necessary to obtain the constitutive equations. The discrete analogue of the balance equation (26) is a frame for the verification of the compatibility and the completeness of these approximations. This problem will be the subject of one of our future papers.

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