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BALANCE EQUATIONS FOR A FINITE NUMBER OF PARTICLES

C. VAMOŞ, A. GEORGESCU and N. SUCIU

In this article an abstract discrete system is considered, consisting of an arbitrary, finite number of particles modelled as mathematical points to which analytic functions of time are attached. We prove that a space-time average of these analytic functions can be defined, satisfying a relation of the same form with the balance equations in continuum mechanics.

1. INTRODUCTION

The balance equations are postulated relations for fundamental physical quantities (mass, momentum, energy, entropy etc.) valid for all continuous media [11]. We take over the differential expression of the balance equations from [9]. Let Ψ be a physical quantity additive with respect to space, associated to a continuous medium. That is, there exists a function ψ of space ($\bar{r}$) and time (t), called the volume density of Ψ, such that, for any volume V, the integral $\int_V \psi d\bar{r}$ 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

$$\partial_t \psi + \sum_{\alpha=1}^{3} \partial_\alpha \left(\Phi_\alpha + \psi v_\alpha \right) - (p+s) = 0 \tag{1}$$

where ∂_t is the temporal derivative, ∂_α is the derivative with respect to the α component of $\bar{r}$, 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 $\bar{\Phi}$, 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 (e.g. [1] – [3]). 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 [4]. So far, these results have been extended to hard sphere fluids, also a very idealized molecular model [5].

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For a more complicated microscopic structure, the existence of the balance equations is implicity *postulated* and the problem of the statistical mechanics is reduced to the calculation of the constitutive equations.

In this article we show that the existence of mathematical relations of the form (1) can be proved in the more general framework of the kinematic description for the microscopic evolution of an arbitrary corpuscular physical system. The position and motion of the microscopic particles can be modelled as mathematical points, and the physical quantities characterizing the particles (mass, momentum, acceleration, kinetic momentum etc.) can be modelled as functions of time. Thus, the differential equations (the dynamic system) corresponding to the microscopic evolution of the corpuscular physical system are not known, but the existence of its solution is postulated.

In the following we shall consider an abstract mathematical model for the kinematic microscopic description discussed above. This mathematical discrete system consists of an arbitrary, finite number of mathematical points to which arbitrary functions of time are associated and it has an abstract nature because there is no physical specification for these time functions. Certainly, for a given corpuscular physical system, the functions of time can represent the mass of the particles, their momentum or any other physical quantity, but in general no specific physical quatity is assigned to the mathematical points. To be more concise, we shall use the name of "particles" or "material points" for these mathematical points together with the assigned abstract functions of time.

The particles can appear or disappear as a result of certain instantaneous processes. Every particle has a temporal interval of existence which can be different from the temporal interval over which we study the discrete system. We assume that a single existence interval corresponds to a given particle, i.e. its disappearance at one time precludes its reappearance. Even if a particle of the same type appears later on, it is considered as a new particle. For the abstract discrete system we do not impose any connection between the disappearance of some particles and the appearance of others. Certainly, in the case of processes like chemical reactions, such connections exist and mass, momentum and energy must be conserved.

The only dynamical requirement is that the evolution of the abstract discrete system (both the variation of the particles position and the associated functions) should be given by analitic functions of time. Under these circumstances we shall prove that a space-time average of the arbitrary functions of time has a.e. continuous partial derivatives. We emphasize that the averaging is an ordinary mathematical one, not a statistical average on an infinite ensemble of identical copies of the physical system. Although these averages preserve the discontinuities associated to the particles as discontinuity surfaces, they satisfy a relation of the form (1). To eliminate and posibility of confusion, we shall call the relations obtained for the abstract discrete system, the "discrete analogue" of the relations of continuum mechanics having a similar form.

We shall apply these results to a Hamiltonian system formed by a single type of particles which neither disappear, nor appear. Every particle is characterized by a constant mass. For this case we shall write the discrete analogue of the balance equations for mass, momentum and energy. We shall briefly discuss the relation with the approach in nonequilibrium statistical mechanics.

2. THE DISCRETE ANALOGUE OF CONTINUOUS FIELDS

We study the evolution during the temporal interval $I = [0,T] \subset \mathbb{R}$ of an abstract discrete system consisting of N particles (i.e. mathematical points with the assigned functions of time). We denote by $I_i = \left[t_i^+, t_i^-\right] \subset I$ the existence inteval of the i-th particle ($1 \le i \le N$). Obviously $0 \le t_i^+ < T$ and $0 < t_i^- \le T$. If $I_i = I$, then the i-th particle exists over the whole interval I. If $I_i \ne I$ for one particle at least, then there are moments when the number of particles is smaller than the total number of particles N. Denoting by $n(t)$ the number of the particles existing at the moment $t \in I$, we have $n(t) \le N$ for each $t \in I$. The equality holds only if $I_i = I$ for all $i \le N$, i.e. if no particles are generated or destroyed over the interval I.

Let $\varphi_i: I \to \mathbb{R}$ be an arbitrary function of time characterizing the i-th particle. If $I_i \ne I$, then $\varphi_i(t) = 0$ for all $t \in I \setminus I_i$. We assume that the restriction $\varphi_i \mid I_i$ can be represented as a Taylor series, i.e. it is an analytic function. In the interval I_i the function 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 $\varphi_i(t_i^+) \ne 0$ and $\varphi_i(t_i^-) \ne 0$, respectively. Similarly, the derivatives of φ_i at t_i^+ and t_i^- may be continuous or discontinuous. The α components of the radius vector $\bar{r}_i$, $x_{\alpha i}: I \to \mathbb{R}$ $(\alpha = 1,2,3)$, and of the velocity $\bar{\xi}_i$, $\xi_{\alpha i}: I \to \mathbb{R}$ $(\alpha = 1,2,3)$ 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.

Definition. For two arbitrary positive real parameters $\tau < T/2$ and a, we define a function $D_\varphi : \mathbb{R}^3 \times (\tau, T-\tau) \to \mathbb{R}$ as

$$\text{(2)} \qquad D_\varphi(\bar{r},t) = \frac{1}{2\tau V} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} \varphi_i(t') H^+\left(a^2 - \left(\bar{r}_i(t') - \bar{r}\right)^2\right) dt'$$

where $V = 4\pi a^3/3$ is the volume of the open sphere of center $\bar{r}$ and radius a denoted by $S(\bar{r}, a)$ and H^+ is the left continuous Heaviside function.

Since $H^+\left(a^2 - \left(\bar{r}_i(t') - \bar{r}\right)^2\right)$ vanishes if the i-th particle is located outside the sphere $S(\bar{r}, a)$ 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 $S(\bar{r}, a)$ over the interval $(t-\tau, t+\tau)$. Therefore $D_\varphi(\bar{r},t)$ characterizes the mean distribution of φ about the point of radius vector $\bar{r}$ at the moment t, and it is a spatial average on the sphere $S(\bar{r}, a)$ and a temporal one over the interval $(t-\tau,\ t+\tau)$. Obviously, it also depends on the parameters τ and a, but we are not interesed in this dependence.

The function $H^{+}\left(a^2-\left(\vec{r}_i(t')-\vec{r}\right)^2\right)$ in (2) takes only the values 0 and 1. The jumps occur when the i-th particle enters or leaves the open sphere $S(\vec{r},a)$. These moments are among the solutions u_i of the equation

$$h_i(\vec{r}_i,u_i)=\left(\vec{r}_i(u_i)-\vec{r}\right)^2-a^2=0 \tag{3}$$

where $\left|h_i(\vec{r},t)\right|^{1/2}$ is the distance at the moment t between the i-th particle and the surface $\partial S(\vec{r},a)$ of the sphere $S(\vec{r},a)$. Since $x_{\alpha i}$, and hence h_i, are analytic functions with respect to u_i, and I_i is a closed interval, then either equation (3) has a finite number of solutions or h_i vanishes identically ([10], p 78). In the latter case the particle moves along the surface of $S(\vec{r},a)$ and does not enter the sphere, hence $H^{+}\left(a^2-\left(\vec{r}_i(t)-\vec{r}\right)^2\right)$ is identically zero and has no jumps. Since $\vec{r}_i(u_i)$ is a known function, then the isolated zeros of (3) are implicit functions $u_i(\vec{r})$. The implicit function theorem can be applied only at interior points and it does not ensure the existence of $u_i(\vec{r})$ for $u_i=t_i^{\pm}$, i.e. $\vec{r}\in\partial S\left(\vec{r}_i(t_i^{\pm}),a\right)$. This case will be discussed separately. For $u_i\in\left(t_i^{+},t_i^{-}\right)$, if

$$\frac{\partial h_i}{\partial u_i}=2\left(\vec{r}_i(u_i)-\vec{r}\right)\cdot\vec{\xi}_i(u_i)\neq 0 \tag{4}$$

then the function $u_i=\vec{r}$ exists in a neighborhood of $\vec{r}$ and has the derivatives

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

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

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

$$\begin{aligned}H^{+}\left(a^2-\left(\vec{r}_i(t)-\vec{r}\right)^2\right)&=H^{+}\left(a^2-\left(\vec{r}_i(t_i^{+})-\vec{r}\right)^2\right)+\\&+\sum_{k'=1}^{n'}H^{+}\left(t-u_{ik'}'\right)-\sum_{k''=1}^{n''}H^{-}\left(t-u_{ik''}''\right)\end{aligned} \tag{6}$$

where H^+ is the right continuous Heaviside jump function. The first term in the right-hand side of (6) vanishes if the i-th particle is generated in the exterior of $S(\bar{r}, a)$ 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 $t_i^+ \le u'_{i1}$ and $u''_{in''} \le t_i^-$. The following notation will be used:

(7) $$U'_i = \left\{u'_{i1}, u'_{i2}, \ldots, u'_{in'}\right\} \text{ and } U''_i = \left\{u''_{i1}, u''_{i2}, \ldots, u''_{in''}\right\}.$$

PROPOSITION 1. *The function D_φ defined by (2) has partial derivatives continuous a.e. in $\mathbb{R}^3 \times (\tau, T-\tau)$.*

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

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

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

(9) $$G_i(\bar{r}, t) = \varphi(t) H^+\left(a^2 - \left(\bar{r}_i(t) - \bar{r}\right)^2\right)$$

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

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

The discontinuities of $\partial_t g_i$ with respect to $(\bar{r}, t)$ 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 i-th particle appears or disappears in $S(\bar{r}, a)$, i.e. $t = t_i^\pm$ and $\bar{r} \in S\left(\bar{r}_i(t_i^\pm), a\right)$, and in the second case the i-th particle lies in the surface of $S(\bar{r}, a)$, i.e. $t \in I_i$ and $\bar{r} \in \partial S\left(\bar{r}_i(t), a\right)$.
Hence the derivative (10) is not continuous over

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

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.

In the appendix we show that the derivative of g_i with respect to x_α exists and is continuous a.e. in $\mathbb{R}^3 \times (\tau, T-\tau)$. Using definition (2) and relations (10), (11), (A3) and (A4), it follows the a.e. continuity of the partial derivatives of D_φ, given by

$$\partial_t D_\varphi(\bar{r},t) = \frac{1}{2\tau V}\sum_{i=1}^{N}\left[G_i(\bar{r},t+\tau) - G_i(\bar{r},t-\tau)\right] \tag{12}$$

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

$$\partial_\alpha D_\varphi(\bar{r},t) = \frac{1}{2\tau V}\sum_{i=1}^{N}\sum_{u\in U_i}\varphi_i(u)\frac{x_{\alpha i}(u) - x_\alpha}{\left|\left(\bar{r}_i(u) - \bar{r}\right)\cdot\bar{\xi}_i(u)\right|} \tag{13}$$

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

3. THE DISCRETE ANALOGUE OF BALANCE EQUATION

PROPOSITION 2. *When the derivatives* (12) *and* (13) *exist, the function* D_φ *satisfies the following relation*

$$\partial_t D_\varphi + \sum_{\alpha=1}^{3}\partial_\alpha D_{\varphi\xi_\alpha} = D_{\dot\varphi} + \left(\partial_t D_\varphi\right)_g \tag{14}$$

where $\left(\partial_t D_\varphi\right)_g$ *is determined by the particles generation.*

Proof. 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 ([8], p331). 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 (12), it follows that $\partial_t D_\varphi$ can also be written as a two term sum

$$\partial_t D_\varphi = \left(\partial_t D_\varphi\right)' + \left(\partial_t D_\varphi\right)'' \tag{15}$$

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

$$G_i'(\bar{r},t+\tau) - G_i'(\bar{r},t-\tau) = \int_{t-\tau}^{t+\tau}\dot\varphi_i(t')H^+\left(a^2 - \left(\bar{r}_i(t') - \bar{r}\right)^2\right)\mathrm{d}t' . \tag{16}$$

Dividing (16) by $2\tau V$, summing up with respect to i, taking into account (9), (12) and (2) we obtain

$$\left(\partial_t D_\varphi\right)' = D_{\dot\varphi} . \tag{17}$$

From (12), the discontinuous part of $\partial_t D_\varphi$ can be written as

$$(18)\qquad \left(\partial_t D_\varphi\right)''(\bar{r},t)=\frac{1}{2\tau V}\sum_{i=1}^{N}\left[G_i''(\bar{r},t+\tau)-G_i''(\bar{r},t-\tau)\right].$$

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 occuring 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 $S(\bar{r},a)$ during the temporal interval $(t-\tau,t+\tau)$. Hence the jump of G_i is equal to

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

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

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

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

$$(19)\qquad G_i''(\bar{r},t+\tau)-G_i''(\bar{r},t-\tau)=\Delta^+G_i+\Delta^-G_i+\sum_{u\in W_i'}\varphi_i(u)-\sum_{u\in W_i''}\varphi_i(u)$$

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 $S(\bar{r},a)$, and it is given by the sign of the expression $-\left(\bar{r}_i(u)-\bar{r}\right)\cdot\bar{\xi}_i(u)$ which is proportional to the interior normal component of $\bar{\xi}_i$ to the surface of $S(\bar{r},a)$ at the moment u. Hence we may use a single sum in (19) if we denote $U_i=W_i'\cup W_i''$. Replacing (19) in (18) we obtain

$$(20)\qquad \left(\partial_t D_\varphi\right)''=\left(\partial_t D_\varphi\right)_g-\frac{1}{2\tau V}\sum_{i=1}^{N}\sum_{u\in U_i}\varphi_i(u)\frac{\left(\bar{r}_i(u)-\bar{r}\right)\cdot\bar{\xi}_i(u)}{\left|\left(\bar{r}_i(u)-\bar{r}\right)\cdot\bar{\xi}_i(u)\right|}$$

where

$$(21)\qquad \left(\partial_t D_\varphi\right)_g=\frac{1}{2\tau V}\sum_{i=1}^{N}\left(\Delta^+G_i+\Delta^-G_i\right).$$

Since $\varphi_i(t)$ and $\xi_{i\alpha}(t)$ are analytic functions with respect to time, then their product is also analytic and relation (20) can be written as

$$(22)\qquad \left(\partial_t D_\varphi\right)''=-\sum_{\alpha=1}^{3}\partial_\alpha D_{\varphi\xi_\alpha}+\left(\partial_t D_\varphi\right)_g.$$

The physical quantity $\varphi_i\bar{\xi}$ represents the transport of φ by the i-th particle, and the space-time average $D_{\varphi\bar{\xi}}$ represents the mean flux of φ.

Relation (14) follows from (15), (17) and (22).

In contrast to balance equation (1), relation (14) does not contain a quantity equivalent to the velocity $\bar{v}$. 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 $i\le N$. Since D_1 characterizes the average number of particles per unit volume, the discrete average of φ is defined as

$$\bar{\varphi}(\bar{r},t)=D_\varphi(\bar{r},t)/D_1(\bar{r},t) \tag{23}$$

if $D_1(\bar{r},t)\neq 0$ and it vanishes if $D_1(\bar{r},t)=0$. It is easy to show that $\bar{\bar{\varphi}}=\bar{\varphi}$, $\overline{\varphi_1+\varphi_2}=\bar{\varphi}_1+\bar{\varphi}_2$ and $\overline{\lambda\varphi}=\lambda\bar{\varphi}$, where λ is a real function of $\bar{r}$ and t.

The mean motion of the particle is given by the discrete average of the velocity $\bar{\bar{\xi}}$ with the components $\bar{\xi}_\alpha$. To introduce $\bar{\xi}_\alpha$ in (14), we write

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

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

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

$\bar{e}_\alpha$ being the unit vectors in ordinary three-dimensional space. Then (14) becomes

$$\partial_t D_\varphi+\nabla\cdot\left(D_\varphi\bar{\bar{\xi}}\right)+\nabla\cdot\bar{\Phi}'_\varphi=D_{\dot{\varphi}}+\left(\partial_t D_\varphi\right)_g \tag{24}$$

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

4. THE HAMILTONIAN SYSTEMS

In this section we consider a Hamiltonian system consisting of a single type of particles. The abstract particles considered till now become real particles with mass m, satisfying the principles of classical mechanics. Obviously, the mass m is constant in time and the same for all the particles. Since we have a single type of particles which are not generated or destroyed, the generating term (21) vanishes.

The relation (24) for mass is obtained if $\varphi_i(t)=m$ for all $t\in I_i$ and $i\le N$. Then $D_\varphi=D_m=mD_1$ is the discrete analogue of the mass density. Moreover, $\bar{\varphi}=m$, $\bar{\Phi}'_m=0$, $\dot{\varphi}_i=0$ and (24) becomes the discrete analogue of the continuity equation

$$\partial_t D_m+\nabla\cdot\left(D_m\bar{\bar{\xi}}\right)=0\,. \tag{25}$$

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

$$\sigma'_{\alpha\beta} = -\left(\bar{\Phi}'_{p_\alpha}\right)_\beta = -\frac{m}{2\tau V}\sum_{i=1}^{N}\int_{t-\tau}^{t+\tau}\left(\xi_{\alpha i}(t') - \bar{\xi}_\alpha\right)\left(\xi_{\beta i}(t') - \bar{\xi}_\beta\right)\cdot \tag{26}$$

$$\cdot H'\left(a^2 - \left(\bar{r}_i(t') - \bar{r}\right)^2\right)dt'$$

The derivative $\dot{\varphi}_i$ is the a component of the force $\bar{f}_i$ acting on the i-th particle and relation (24) becomes

$$\partial_t\left(D_m\bar{\xi}_\alpha\right) + \sum_{\beta=1}^{3}\partial_\beta\left(D_m\bar{\xi}_\alpha\bar{\xi}_\beta\right) - \sum_{\beta=1}^{3}\partial_\beta\sigma'_{\alpha\beta} = D_{f_\alpha} \tag{27}$$

Making additional hypotheses on the interaction between particles, one can prove that equation (27) is the discrete analogue of the momentum equation in continuum mechanics [7].

Choosing as physical quantity the kinetic energy of the particles $\varphi_i = E_i = \frac{1}{2}m\xi_{p_i}^2$, we obtain

$$D_E = \frac{1}{2}mD_{\left[\bar{\xi}+(\xi-\bar{\xi})\right]^2} = \frac{1}{2}mD_{\bar{\xi}^2} + \frac{1}{2}mD_{\bar{\xi}(\xi-\bar{\xi})} + \frac{1}{2}mD_{(\xi-\bar{\xi})^2}$$

where we used the linearity of D_φ with respect to φ, i.e. $D_{\varphi_1+\varphi_2} = D_{\varphi_1} + D_{\varphi_2}$. The second term of the expression vanishes $D_{\bar{\xi}(\xi-\bar{\xi})} = \bar{\bar{\xi}}\cdot D_{\xi-\bar{\xi}} = \bar{\bar{\xi}}\cdot\left(D_\xi - D_{\bar{\xi}}\right) = 0$. The last term is the discrete analogue of the kinetic energy density of the thermal motion, since $\frac{1}{2}m\left(\bar{\xi} - \bar{\bar{\xi}}\right)^2$ represents the kinetic energy of the relative motion of the i-th particle with respect to the mean motion of the particles in the sphere $S(\bar{r}, a)$, over $(t-\tau, t+\tau)$. We denote this term by

$$\varepsilon = \frac{1}{2}mD_{(\xi-\bar{\xi})^2} = \frac{1}{2}\sum_{\alpha=1}^{3}\sigma'_{\alpha\alpha}$$

the last equality following directly from (26). Similarly

$$\left(\bar{\Phi}_E\right)_\alpha = \frac{1}{2}mD_{\xi^2(\xi_\alpha-\bar{\xi}_\alpha)} = \frac{1}{2}\sum_{\beta=1}^{3}\xi_\beta\sigma'_{\alpha\beta} + \left(\bar{\Phi}_\varepsilon\right)_\alpha$$

where the flux of the discrete analogue of the kinetic energy of the thermal motion is

$$\bar{\Phi}_\varepsilon = \frac{1}{2}mD_{(\xi-\bar{\xi})^2(\xi-\bar{\xi})}.$$

The time derivative of the kinetic energy can not be written in a simple form, so the balance equation (24) for kinetic energy becomes

$$(28)\quad \partial_t\left(\frac{1}{2}D_m\overline{\overline{\xi}}^2+\varepsilon\right)+\nabla\cdot\left[\left(\frac{1}{2}D_m\overline{\overline{\xi}}^2+\varepsilon\right)\overline{\overline{\xi}}\right]+\nabla\cdot\vec{\Phi}_\varepsilon+\sum_{\alpha,\beta=1}^{3}\partial_\alpha\left(\overline{\xi_\beta\sigma'_{\alpha\beta}}\right)=D_E\,.$$

In addition to relations (25), (27) and (28), discrete analogues of balance equations for any physical quantity are possible.

5. CONCLUSION

Relation (24) is not a balance equation, but an identity *of the same form* with a balance equation. It has been derived under general conditions, for an arbitrary, finite number of mathematical points to which analytic functions of time were attached. Due to this very general approach, the results can be applied to a large number of corpuscular physical systems. For example, the discrete analogue of the balance equation (24) is valid for an arbitrary physical quantity, and for an arbitrary number of particles (even very small). Also, since the dynamical equations for the microscopic evolution have not been used explicity, relation (24) holds for any microscopic interaction forces satisfying the analycity condition. In this article we have considered the case of the Hamiltonian systems consisting of a single type of particles which can not be generated or destroyed.

To transform the function D_φ defined by (2) into a continuous field, and relation (24) into a balance equation, a statistical average on an ensemble formed by a very large number of identical copies of the considered corpuscular system is needed. Although, if the number of particles contributing to the value of D_φ is large enough, then D_φ approximates closely the continuous field corresponding to the physical quantity φ. That is, if the physical system satisfies the local equilibrium principle [6], then the parameters a and τ can be chosen so that the particles lying in the sphere $S(\vec{r}\,,a)$ over the interval $(t-\tau,\, t+\tau)$ should form a near-equilibrium thermodynamical system [12]. Obviously, in this case the total number of particles N can no longer be arbitrary, but it must be large enough to ensure the validity of the thermodynamical limit.

The balance equation in continuum mechanics can also be obtained as the limit for $a\to 0$ and $\tau\to 0$ of the statistical average of relation (24). Both methods to obtain the balance equation (1) from (24) will be discuss in another article.

APPENDIX

Here we study the differentiability with respect to $\vec{r}$ of the function g_i defined by (8). Although (6) holds only for $t\in I_i$, it may be substituted in (8) because φ_i

vanishes for $t \in I \setminus I_i$, and we obtain

$$\text{(A1)}\quad g_i(\vec{r},t) = H^+\left(a^2 - \left(\vec{r}_i\left(t_i^+\right) - \vec{r}\right)^2\right)\int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right)\mathrm{d}t' + \sum_{u \in U_i'} \int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right) H^+\left(t'-u\right)\mathrm{d}t' -$$

$$-\sum_{u \in U_i''} \int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right) H^-\left(t'-u\right)\mathrm{d}t'$$

where U_i' and U_i'' are defined in (7). First, we consider $2\tau < t_i^- - t_i^+$. The following cases are possible:

(a) $t \le t_i^+ - \tau$. Then $(t-\tau, t+\tau) \cap I_i = \varnothing$ and φ_i vanishes in the integration intervals in (A1), such that $g_i(\vec{r},t) = 0$ for all $\vec{r} \in \mathbb{R}^3$.

(b) $t \in \left(t_i^+ - \tau, t_i^+ + \tau\right]$. Then $(t-\tau, t+\tau) \cap I_i = \left[t_i^+, t+\tau\right)$ and the integral in (A1) have the same limits. The first term in (A1) depends on $\vec{r}$ through the function $H^+\left(a^2 - \left(\vec{r}_i\left(t_i^+\right) - \vec{r}\right)^2\right)$ which can take only the values 0 and 1. Hence, when this function is continuous with respect to $\vec{r}$, its derivative exists and equals zero. Then the first term in (A1) is not differentiable if $H^+\left(a^2 - \left(\vec{r}_i\left(t_i^+\right) - \vec{r}\right)^2\right)$ is discontinuous, i.e. $\vec{r} \in \partial S\left(\vec{r}_i\left(t_i^+\right), a\right)$. The others terms in (A1) depend on $\vec{r}$ through the moments u defined by (3). These terms are not differentiable either if u is not differentiable (i.e. relation (4) is not satisfied) of if the moments u coincide with the integration limits (i.e. $\vec{r} \in \partial S\left(\vec{r}_i\left(t_i^+\right), a\right)$ or $\vec{r} \in \partial S\left(\vec{r}_i(t+\tau), a\right)$). In this case the integration intervals have discontinuous variations with respect to $\vec{r}$.

(c) $t \in \left(t_i^+ + \tau, t_i^- - \tau\right)$. Then $(t-\tau, t+\tau) \cap I_i = (t-\tau, t+\tau)$ and the integrals with $u \le t-\tau$ are equal to the integral of the first term. Using the expression

$$H^+\left(a^2 - \left(\vec{r}_i\left(t_i^+\right) - \vec{r}\right)^2\right) + \sum_{u \in W_1'} H^+(t-u) - \sum_{u \in W_1''} H^{-}(t-u) = H^+\left(a^2 - \left(\vec{r}_i(t-\tau) - \vec{r}\right)^2\right)$$

where $W_1' = U_i' \cap \left[t_i^+, t-\tau\right]$ and $W_1'' = U_i'' \cap \left(t_i^+, t-\tau\right]$, relation (A1) becomes

$$\text{(A2)}\quad g_i(\vec{r},t) = H^+\left(a^2 - \left(\vec{r}_i(t-\tau) - \vec{r}\right)^2\right)\int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right)\mathrm{d}t' + \sum_{u \in W_2'} \int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right) H^+\left(t'-u\right)\mathrm{d}t' -$$

$$-\sum_{u \in W_2''} \int_{t-\tau}^{t+\tau} \varphi_i\left(t'\right) H^-\left(t'-u\right)\mathrm{d}t'$$

where $W_2' = U_i' \cap \left(t-\tau, t_i^-\right)$ and $W_2'' = U_i'' \cap \left(t-\tau, t_i^-\right]$. As for (b), the first term is not differentiable if $\vec{r} \in \partial S\left(\vec{r}_i(t-\tau), a\right)$ and the other terms if $\vec{r} \in \partial S\left(\vec{r}_i(t+\tau), a\right)$, or if relation (4) is not satisfied.

(d) $t\in\left[t_i^- -\tau, t_i^- +\tau\right)$. Then $(t-\tau,t+\tau)\cap I_i=\left(t-\tau,t_i^-\right]$ and the expression for $g_i(\bar{r},t)$ is identic with (A2), except the upper integration limit is t_i^- . So $g_i(\bar{r},t)$ is not differentiable if $\bar{r}\in\partial S\left(\bar{r}_i(t-\tau),a\right)$ or $\bar{r}\in\partial S\left(\bar{r}_i\left(t_i^-\right),a\right)$ or (4) is not satisfied.

(e) $t\ge t_i^- +\tau$. Then $(t-\tau,t+\tau)\cap I_i=\varnothing$ and $g_i(\bar{r},t)=0$.

If $\tau<t_i^- -t_i^+<2\tau$, then the possible cases for (A1) are $t\le t_i^+ -\tau$, $t\in\left(t_i^+ -\tau,t_i^- -\tau\right)$, $t\in\left[t_i^- -\tau,t_i^+ +\tau\right]$, $t\in\left(t_i^+ +\tau,t_i^- +\tau\right)$ and $t\ge t_i^- +\tau$ and the discussion is similar. Finally, if $t_i^- -t_i^+\le\tau$, then other five intervals for t exist. Taking into account that $t\in(\tau, T-\tau)$, the set where the function g_i is not differentiable with respect to $\bar{r}$ is

$$
\begin{aligned}
\text{(A3)}\qquad \Omega_i'' = &\left\{(\bar{r},t)\middle| t\in\left(t_i^+ -\tau,t_i^+ +\tau\right]\cap(\tau,T-\tau)\text{ and }\bar{r}\in\partial S\left(\bar{r}_i\left(t_i^+\right),a\right)\right\}\cup\\
&\cup\left\{(\bar{r},t)\middle| t\in\left[t_i^- -\tau,t_i^- +\tau\right)\cap(\tau,T-\tau)\text{ and }\bar{r}\in\partial S\left(\bar{r}_i\left(t_i^-\right),a\right)\right\}\cup\\
&\cup\left\{(\bar{r},t)\middle| t\in\left(t_i^+ \pm\tau,t_i^- \pm\tau\right)\cap(\tau,T-\tau)\text{ and }\bar{r}\in\partial S\left(\bar{r}_i(t\mp\tau),a\right)\right\}\cup\\
&\cup\left\{(\bar{r},t)\middle| t\in(\tau,T-\tau),\text{ exists } t'\in(t-\tau,t+\tau)\cap I_i \text{ such that}\right.\\
&\left.\bar{r}\in\partial S\left(\bar{r}_i\left(t'\right),a\right)\text{ and }\left(\bar{r}_i\left(t'\right)-\bar{r}\right)\cdot\bar{\xi}_i\left(t'\right)=0\right\}
\end{aligned}
$$

This is a set of null Lebesgue measure in $\mathbb{R}^3\times(\tau, T-\tau)$.

Only the terms in (A1) which contain u in the integration interval have a nonvanishing contribution to the derivative of g_i with respect to x_α, denoted by $\partial_\alpha g_i$. Using (5) and taking into account that the sign of the terms in (A1) coincides with the sign of the expression $-\left(\bar{r}_i(u)-\bar{r}\right)\cdot\bar{\xi}_i(u)$, we obtain

$$
\text{(A4)}\qquad \partial_\alpha g_i(\bar{r},t)=\sum_{u\in U_i}\varphi_i(u)\frac{x_{\alpha i}(u)-x_\alpha}{\left|\left(\bar{r}_i(u)-\bar{r}\right)\cdot\bar{\xi}_i(u)\right|}
$$

where $U_i=\left(U_i'\cup U_i''\right)\cap(t-\tau,t+\tau)$. It is obvious that $\partial_\alpha g_i$ is continuous over $\mathbb{R}^3\times(\tau,T-\tau)\setminus\Omega_i''$.

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Romanian Academy
Institute of Applied Mathematics
P. O. Box 1-24, 70700 Bucharest 1
Romania