Chapter 4

Coarse-grained averages

4.1 The concentration definition

As we said in the chapter 2, the derivation of the balance equations starting from the kinematic microscopic description of the corpuscular system is based on the utilization of the space-time coarse-grained averages. The necessity to introduce the combination between a space averaging and a time one in order to define the macroscopic quantities as a consequence of the measuring processes has been shown ever since 1946 by Kirkwood [27]: "In measuring the macroscopic observables one not only takes a statistical average over the systems of an ensemble (by repeating the observations many times) but two additional averages as well. The first is a spatial average over a microscopically large though macroscopically small domain, determined by the resolving power of one's measuring instruments. The second is a time average over an interval determined by the relaxation time of one's measuring instruments." The difference from our approach consists in the fact that Kirkwood's time average of the probability distribution is defined in the phase space and not the quantities in the three-dimensional physical space.

In order to present the physical significance of the space-time coarse-grained average we discuss in detail the definition of the concentration. Consider N molecules in a volume V. The concentration at the point with the radius vector $\mathbf{r}$ at time t is defined as the number of particles per unit volume in a domain of volume $\mathcal{V} < V$ centered at this point. The domain with the volume $\mathcal{V}$ should be spherical, otherwise the concentration would depend not only on the position but also on the orientation of the domain. We denote by $S(\mathbf{r}, a)$ the sphere with center $\mathbf{r}$ and radius a. Then the concentration is

defined as the function $c : \mathbf{R}^3 \times \mathbf{R} \to \mathbf{R}_+$ given by

$$c(\mathbf{r}, t) = \frac{1}{\mathcal{V}} \sum_{i=1}^{N} H^+(a^2 - (\mathbf{r}_i(t) - \mathbf{r})^2) \tag{4.1}$$

where $\mathbf{r}_i(t)$, $t \in \mathbf{R}$, is the radius vector of the molecule $i \leq N$ at time t. The left continuous Heaviside function $H^+(a^2 - (\mathbf{r}_i(t) - \mathbf{r})^2)$ is equal to 1 if the molecule i is inside the interior of the sphere $S(\mathbf{r}, a)$ and vanishes otherwise. The function defined by (4.1) for given a and $\mathbf{r}_i$, is a finite linear combination of Heaviside functions having null derivatives except when their argument vanishes and the derivatives does not exist. Hence (4.1) defines a step function which cannot satisfy a partial derivative equation of the type of the diffusion equation (1.5). It can, at the most, approximate the actual concentration which obeys the diffusion equation. The approximation is better if the number of molecules N increases because then the steps of the function (4.1) are smaller.

However in thermodynamics one considers that a continuous field of the concentration exists and it is obtained from $c(\mathbf{r}, t)$ given by (4.1) if N is large enough. To obtain the condition that N should satisfy we analyze the simple case of the thermodynamical equilibrium state in absence of the exterior fields. Then the molecules are uniformly distributed in the volume V and, taken as a continuous field, the concentration has a constant value at any point in the volume and at moment, $c_o(\mathbf{r}, t) = N/V$. If we want to verify this equilibrium distribution by means of the definition (4.1), we count the number of molecules n at the moment t in the sphere $S(\mathbf{r}, a)$. It is obviously that the result is affected by fluctuations and the measured concentration $c(\mathbf{r}, t) = n/\mathcal{V}$ differs from c_o. In fact n and in consequence $c(\mathbf{r}, t)$ are random variables. In [40], Section 114 , it is proved that n satisfy a Poisson distribution with standard deviation $\sigma = \sqrt{\overline{n}}$, where $\overline{n} = N\mathcal{V}/V$ is the mean number of molecules in $\mathcal{V}$. Hence the standard deviation of the concentration is equal to $\sigma_c = \sigma/\mathcal{V} = \sqrt{N\,/\,(V\mathcal{V})}$. If N is large enough, $\Delta c = c - c_o$ has a normal distribution with zero mean and standard deviation σ_c. According to the "three sigma" of exclusion of the rough errors [50], we impose the condition that the relative error be smaller than a fixed value ε with a confidence level of $0,997$

$$3\sigma_c \leq \varepsilon c_o$$

and we obtain

$$\frac{\mathcal{V}}{V} \geq \frac{9}{\varepsilon^2 N} \,. \tag{4.2}$$

For given N, this formula gives the minimum volume $\mathcal{V}$ (or the minimum radius a) necessary to measure the concentration with the precision ε, i.e., the space scale for which the measured concentration behaves like a continuous field with the approximation ε. Hence, if (4.2) is satisfied, we can write $c(\mathbf{r},t) \sim c_o(\mathbf{r},t) + \mathcal{O}(\varepsilon)$, for $\varepsilon \to 0$.

The classical definition of the concentration (4.2) is not applicable when N or $\mathcal{V}$ is too small. To exemplify, we consider the case when there is a single molecule in the volume V. Then $c(\mathbf{r},t) = \mathcal{V}^{-1}$ in the interior of the sphere with radius a centred on the molecule, i.e., for $\mathbf{r} \in S(\mathbf{r}_1(t),a)$, and in rest c vanishes. Therefore the concentration is completely different from the equilibrium concentration $c_o(\mathbf{r},t) = 1/V$ in the entire volume V. These difficulties occur because in the definition (4.1) it is implicitly supposed an instantaneous measurement of the number of molecules in the volume $\mathcal{V}$. In fact, as Kirkwood noticed, any measurement has a duration which defines the time scale of the continuous description, in the same way as the volume $\mathcal{V}$ (or the radius a) define the spatial scale. If we denote by $(t-\tau, t+\tau)$ the averaging interval, we define the concentration by

$$c(\mathbf{r},t) = \frac{1}{2\tau\mathcal{V}} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2) dt' \ . \tag{4.3}$$

In the next sections we prove that the function (4.3) has a.e. continuous first order partial derivatives. That is, the time averaging transforms the step function (4.1) into a continuous field even the discontinuities are preserved in the first order partial derivatives.

The new definition (4.3) is meaningful even when $\mathcal{V}$ or N is very small and the classical definition (4.1) cannot be applied. Consider again the thermodynamical equilibrium state with a uniform distribution of the molecules in the volume V. The number of molecules in $\mathcal{V}$ is measured at each moment over the interval $(t-\tau, t+\tau)$ and then it is averaged. In order to obtain a simple estimation of the magnitude order of the fluctuations of the concentration (4.3) with respect to the equilibrium concentration $c_o(\mathbf{r},t)$, we associate to this continuous time average a discrete one, to which we can apply the same Poisson distribution. We denote by $\triangle t$ the mean interval over which the molecule remains inside the volume $\mathcal{V}$. We divide the averaging interval $(t-\tau, t+\tau)$ in $2\tau/\triangle t$ subintervals of length Δt. As we only want to obtain some indications on the magnitude order of the fluctuations, we suppose that the existence of the molecule in the volume $\mathcal{V}$ during a subinterval $\triangle t$ is independent from its existence in the same volume during another subinterval $\triangle t$. Then the concentration fluctuations (4.3) for N molecules over a time

interval of length 2τ, are equivalent to the fluctuations of $2N\tau/\triangle t$ molecules over an interval $\triangle t$. Therefore instead the formula (4.2) we have

$$\frac{\mathcal{V}}{V} \geq \frac{9}{\varepsilon^2} \cdot \frac{\triangle t}{2\,N\,\tau}\,,$$

or

$$\mathcal{V}\tau \geq \frac{9\triangle t}{2\varepsilon^2 c_o}\,. \tag{4.4}$$

This formula expresses the relation between the space scale ($\mathcal{V}$) and the temporal one (τ), necessary to obtain a continuous description of the concentration with precision ε. Unlike (4.1), the relation (4.3) is valid for any N. For example, let us apply (4.4) for $N = 1$, that is $c_o = V^{-1}$. For any value of the volume $\mathcal{V}$, there is a τ large enough such that (4.4) is satisfied and the measurement result is a concentration equal with c_o with the approximation ε. Thus (4.3) removes the restriction of the definition (4.1) for small number of particles. This is possible because the increase of the time scale can compensate the decrease of the space scale.

Also we notice that the integral with respect to time in (4.3) is identical with that used in the formulation of the ergodic hypothesis. Hence for nonvanishing τ, more microstates of the corpuscular system are included into $c(\mathbf{r}, t)$. Therefore the smoothness of $c(\mathbf{r}, t)$ is better in comparison with the instantaneous spatial average (4.1). If the corpuscular system is in a stationary state, then we can consider $\tau \to \infty$ and the spatial averaging can be performed on a no matter how small volume, even reduced to a point ($a \to 0$). For the nonstationary processes the upper limit of τ is given by the magnitude order of the time intervals in which the physical quantities have important variations.

A coarse-grained averaging very similar to (4.3) is used in the molecular dynamics in order to obtain a macroscopic description attached to a numerical simulation of the evolution of an ensemble of hundreds or thousands molecules [35]. The main difference is that the averaging space domain does not have a well-defined form. That is why one cannot prove that the coarse-grained average satisfies a relation of the balance equation form.

Another attempt to obtain the continuous description starting from a space-time coarse-grained average can be found in [47] and [48]. Similarly to our method, the local equilibrium principle is used to smooth the microscopic discontinuities. The main difference is that we smooth the discontinuities *after* a relation of the balance equation form was obtained. Similarly to the usual statistical method, Murdoch obtains *in the same time* both the balance equations and the smoothness characteristic to the macroscopic continuous

fields. Furthermore, he is compelled to use different hypotheses on the interaction forces between the molecules in order to obtain the usual equations in continuum mechanics.

4.2 The coarse-grained average definition

In the previous chapter we have presented the derivation of the balance equations in the statistical mechanics when it is assumed that the motion of the component particles is described by a Hamiltonian dynamical system. In this chapter we use only the kinematic description presented in the chapter 2, for which this assumption is not necessary. We show that the space-time coarse-grained average of an arbitrary physical quantity has almost everywhere continuous partial derivatives. We emphasize that the coarse-grained average is not a statistical average on an infinite ensemble of identical representatives of a physical system. Although the coarse-grained averages preserve the discontinuities of the discrete microscopic structure as discontinuity surfaces, they satisfy a relation of the form of the balance equations. In order to eliminate possible confusions, the relations obtained for the abstract discrete system defined in section 1.2., will be called "the discrete analogue" of the relations with similar form in continuum mechanics. The results obtained in this chapter have been published in [63] and [64].

Using the notation and definitions in Chapter 2, we generalize the relation (4.3).

Definition *For two arbitrary positive real parameters $\tau < T/2$ and a, we define the function $\langle\varphi\rangle : \mathbf{R}^3 \times (\tau, T-\tau) \to \mathbf{R}$*

$$\langle\varphi\rangle(\mathbf{r},t) \;=\; \frac{1}{2\tau\mathcal{V}} \sum_{i=1}^{N} \int_{t-\tau}^{t+\tau} \varphi_i(t')\, H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2)\, dt', \qquad (4.5)$$

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

Since $H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2)$ vanishes if the i-th particle is located outside the sphere $S(\mathbf{r}, a)$ and $\varphi_i(t')$ vanishes if $t' \in I \setminus I_i$, then a nonvanishing contribution to $\langle\varphi\rangle$ have only the particles lying over the interval $(t-\tau, t+\tau)$ in $S(\mathbf{r}, a)$. Therefore $\langle\varphi\rangle(\mathbf{r}, t)$ characterizes the mean distribution of φ about the point of radius vector $\mathbf{r}$ at the moment t, and it is a spatial average over the sphere $S(\mathbf{r}, a)$ and a temporal over the interval $(t-\tau, t+\tau)$. Then, equation (4.5) defines a *space-time coarse-grained average* with the space scale

given by a and the time scale by τ. Obviously, $\langle\varphi\rangle$ also depends on the parameters τ and a, but we do not explicitly indicate this dependence by notation.

The function $H^+(a^2-(\mathbf{r}_i(t')-\mathbf{r})^2)$ in (4.5) takes only the values 0 and 1. The jumps occur when the i-th particle enters or leaves the open sphere $S(\mathbf{r},a)$. These moments are among the solutions u_i of the equation

$$h_i(\mathbf{r},u_i) \equiv (\mathbf{r}_i(u_i)-\mathbf{r})^2-a^2 = 0, \tag{4.6}$$

where $\mid h_i(\mathbf{r},t) \mid^{1/2}$ is the distance at the moment t between the particle i and the surface $\partial S(\mathbf{r},a)$ of the sphere $S(\mathbf{r},a)$. Since the components $x_{\alpha i}$ of $\mathbf{r}_i$, and hence h_i, are analytic functions with respect to u_i, and I_i is a closed interval, then either the equation (4.6) has a finite number of solutions, or h_i identically vanishes ([56], p. 78). In the latter case the particle moves along the surface of $S(\mathbf{r},a)$ and does not enter the sphere, hence $H^+(a^2-(\mathbf{r}_i(t)-\mathbf{r})^2)$ is identically zero and has no jumps. Since $\mathbf{r}_i(u_i)$ is a known function, then the isolated zeros of equation (4.6) are implicit functions $u_i(\mathbf{r})$. The implicit function theorem can be applied only at interior points, so it does not ensure the existence of $u_i(\mathbf{r})$ for $u_i=t_i^{\pm}$, i.e., for $\mathbf{r}\in\partial S(\mathbf{r}_i(t_i^{\pm}),a)$. This situation will be discussed separately. For $u_i\in(t_i^+,t_i^-)$, if

$$\frac{\partial h_i}{\partial u_i} = 2\,(\mathbf{r}_i(u_i)-\mathbf{r})\cdot\boldsymbol{\xi}_i(u_i) \neq 0, \tag{4.7}$$

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

$$\frac{\partial u_i}{\partial x_\alpha} = -\frac{\partial h_i}{\partial x_\alpha}\Big/\frac{\partial h_i}{\partial u_i} = \frac{x_{\alpha i}(u_i)-x_\alpha}{(\mathbf{r}_i(u_i)-\mathbf{r})\cdot\boldsymbol{\xi}_i(u_i)}\ ,\ \alpha=1,2,3\ . \tag{4.8}$$

According to (4.7), the function $u_i(\mathbf{r})$ is not differentiable at the point of the discriminant surface of the family $\{\partial S(\mathbf{r}_i(t),a);t\in I_i\}$.

For $t=t_i^+$ the function $H^+(a^2-(\mathbf{r}_i(t)-\mathbf{r})^2)$ vanishes if the particle i is generated outside $S(\mathbf{r},a)$ and takes the value 1 otherwise. For $t>t_i^+$ the value of this function has jumps between 0 and 1 at the moments when the particle i intersects the surface of the sphere $S(\mathbf{r},a)$. Since the zeros of the equation (4.6) are in finite number we can denote by $t_i^+<u'_{i1}<u'_{i2}<...<u'_{in'}<t_i^-$ ($t_i^+<u''_{i1}<u''_{i2}<...<u''_{in''}<t_i^-$) the moments when the particle i enters (leaves) the sphere $S(\mathbf{r},a)$. Since the sphere$S(\mathbf{r},a)$ is open, $H^+(a^2-(\mathbf{r}_i(t)-\mathbf{r})^2)$ as a function of t is left (right) continuous when the particle enters (leaves). Hence for $t\in I_i$, we have

$$H^+(a^2-(\mathbf{r}_i(t)-\mathbf{r})^2)=H^+(a^2-(\mathbf{r}_i(t_i^+)-\mathbf{r})^2)+\sum_{k'=1}^{n'}H^+(t-u'_{ik'})-\sum_{k''=1}^{n''}H^-(t-u''_{ik''}), \tag{4.9}$$

where H^- is the right continuous Heaviside function. If $u_i = t_i^+$, the particle can only enter the sphere after its generation, hence $u'_{i1} = t_i^+$ and relation (4.9) holds. If $u_i = t_i^-$, the particle could only leave the sphere before its disappearance, hence $u''_{in''} = t_i^-$ and relation (4.9) holds again. So (4.9) contains all the possible situations if we take $t_i^+ \leq u'_{i1}$ and $u''_{in''} \leq t_i^-$. In the following we use the notation:

$$U'_i \;=\; \{u'_{i1}, u'_{i2}, ..., u'_{in'}\} \quad \text{and} \quad U''_i \;=\; \{u''_{i1}, u''_{i2}, ..., u''_{in''}\}. \tag{4.10}$$

We want to prove that the function $\langle\varphi\rangle$ defined by (4.5) has partial derivatives continuous a.e. in $R^3 \times (\tau, T-\tau)$. To study the differentiability of $\langle\varphi\rangle$, we consider the function $g_i : \mathbf{R}^3 \times (\tau, T-\tau) \to \mathbf{R}$

$$g_i(\mathbf{r}, t) \;=\; \int_{t-\tau}^{t+\tau} \varphi_i(t')\, H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2)\, dt'. \tag{4.11}$$

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

$$G_i(\mathbf{r}, t) \;=\; \varphi_i(t)\, H^+(a^2 - (\mathbf{r}_i(t) - \mathbf{r})^2) \tag{4.12}$$

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 a partial derivative with respect to t a.e. in $(\tau, T-\tau)$, equal to

$$\partial_t g_i(\mathbf{r}, t) \;=\; G_i(\mathbf{r}, t+\tau) \;-\; G_i(\mathbf{r}, t-\tau). \tag{4.13}$$

The discontinuities of $\partial_t g_i$ with respect to $(\mathbf{r}, t)$ are related to those of G_i. From (4.12) it follows that G_i is discontinuous when φ_i is discontinuous and H^+ nonvanishing, or conversely, if H^+ is discontinuous and φ_i nonvanishing. In the first case the i-th particle appears or disappears in $S(\mathbf{r}, a)$, i.e., $t = t_i^\pm$ and $\mathbf{r} \in S(\mathbf{r}_i(t_i^\pm), a)$, and in the second case the i-th particle lies on the surface of $S(\mathbf{r}, a)$, i.e., $t \in I_i$ and $\mathbf{r} \in \partial S(\mathbf{r}_i(t), a)$. Hence the derivative (4.13) is not continuous on

$$\begin{aligned}
\Omega'_i \;=\; & \{(\mathbf{r}, t) \mid t \in \{t_i^+ - \tau, t_i^+ + \tau\} \cap (\tau, T-\tau) \text{ and } \mathbf{r} \in S(\mathbf{r}_i(t_i^+), a)\} \cup \\
& \{(\mathbf{r}, t) \mid t \in \{t_i^- - \tau, t_i^- + \tau\} \cap (\tau, T-\tau) \text{ and } \mathbf{r} \in S(\mathbf{r}_i(t_i^-), a)\} \cup \\
& \{(\mathbf{r}, t) \mid t \in [t_i^+ + \tau, t_i^- + \tau] \cap (\tau, T-\tau) \text{ and } \mathbf{r} \in \partial S(\mathbf{r}_i(t-\tau), a)\} \cup \\
& \{(\mathbf{r}, t) \mid t \in [t_i^+ - \tau, t_i^- - \tau] \cap (\tau, T-\tau) \text{ and } \mathbf{r} \in \partial S(\mathbf{r}_i(t+\tau), a)\}
\end{aligned} \tag{4.14}$$

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

Although (4.9) holds only that for $t \in I_i$, it may be substituted in (4.11) because φ_i vanishes for $t \in I \setminus I_i$. We obtain

$$g_i(\mathbf{r},t) = H^+(a^2 - (\mathbf{r}_i(t_i^+) - \mathbf{r})^2) \int_{t-\tau}^{t+\tau} \varphi_i(t')\, dt' + \sum_{u \in U_i'} \int_{t-\tau}^{t+\tau} \varphi_i(t') H^+(t'-u) dt' - \sum_{u \in U_i''} \int_{t-\tau}^{t+\tau} \varphi_i(t') H^-(t'-u)\, dt', \qquad (4.15)$$

where U_i' and U_i'' are defined in (4.10). In the following we analyze the differentiability of the function $g_i(\mathbf{r},t)$ with respect to x_α using the expression given by (4.15). Since the function φ_i vanishes outside the interval I_i, the integration interval in (4.15) is equal with $(t-\tau, t+\tau) \cap I_i$. This intersection has a nonvanishing length if $t \in (t_i^+ - \tau, t_i^- + \tau)$. The left endpoint of the intersection is equal to t_i^+ if $t \le t_i^+ + \tau$ and is equal to $t-\tau$ if $t > t_i^+ + \tau$. The right endpoint of the intersection is equal to $t+\tau$ or t_i^- depending if $t < t_i^- - \tau$ or $t \ge t_i^- - \tau$. The variation in terms of t of this intersection depends on the relation between the moments $t_i^+ + \tau$ and $t_i^- - \tau$. First we assume that $t_i^+ + \tau < t_i^- - \tau$, that is $2\tau \le t_i^- - t_i^+$. For the interval $(t-\tau, t+\tau) \cap I_i$ the following situations 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 (4.15), so that $g_i(\mathbf{r},t) = 0$ for all $\mathbf{r} \in \mathbf{R}^3$.

(b) $t \in (t_i^+ - \tau, t_i^+ + \tau]$. Then the integrals from (4.15) have the integration interval $(t-\tau, t+\tau) \cap I_i = [t_i^+, t+\tau)$. The first term in (4.15) depends on $\mathbf{r}$ through the function $H^+(a^2 - (\mathbf{r}_i(t_i^+) - \mathbf{r})^2)$ which can take only the values 0 and 1. So, when this function is continuous with respect to $\mathbf{r}$, its derivative exists and is equal to zero Then the first term in (4.15) is not differentiable if $H^+(a^2 - (\mathbf{r}_i(t_i^+) - \mathbf{r})^2)$ is discontinuous, i.e., $\mathbf{r} \in \partial S(\mathbf{r}_i(t_i^+), a)$. The other terms in (4.15) depend on $\mathbf{r}$ through the moments u defined by (4.6). These terms are not differentiable either if the implicit function $u(\mathbf{r})$ is not differentiable (the relation (4.6) is not satisfied), or if the moments u coincide with the integration limits ($\mathbf{r} \in \partial S(\mathbf{r}_i(t_i^+), a)$ or $\mathbf{r} \in \partial S(\mathbf{r}_i(t+\tau), a)$). In this case the integration intervals have discontinuous variations with respect to $\mathbf{r}$.

(c) $t \in (t_i^+ + \tau, t_i^- - \tau)$. Then $(t-\tau, t+\tau) \cap I_i = (t-\tau, t+\tau)$ and the integrals in (4.15) with $u \le t - \tau$ are equal to the first term. In the same as

we obtained the relation (4.9) we have

$$H^+(a^2-(\mathbf{r}_i(t_i^+)-\mathbf{r})^2)\,+\sum_{u\in W_1'}H^+(t-u)-\quad\sum_{u\in W_1''}H^-(t-u)=\\ H^+(a^2-(\mathbf{r}_i(t-\tau)-\mathbf{r})^2)\ ,$$

where $W_1'=U_i'\cap[t_i^+,t-\tau]$ and $W_1''=U_i''\cap(t_i^+,t-\tau]$. The relation (4.15) becomes

$$g_i(\mathbf{r},t)\ =H^+(a^2-(\mathbf{r}_i(t-\tau)-\mathbf{r})^2)\int_{t-\tau}^{t+\tau}\varphi_i(t')\,dt'+\\ \sum_{u\in W_2'}\int_{t-\tau}^{t+\tau}\varphi_i(t')H^+(t'-u)dt'-\sum_{u\in W_2''}\int_{t-\tau}^{t+\tau}\varphi_i(t')H^-(t'-u)\,dt',\qquad(4.16)$$

where $W_2'=U_i'\cap(t-\tau,t_i^-]$ and $W_2''=U_i''\cap(t-\tau,t_i^-]$. As for **(b)**, the first term is not differentiable if $\mathbf{r}\in\partial S(\mathbf{r}_i(t-\tau),a)$ and the other terms if $\mathbf{r}\in\partial S(\mathbf{r}_i(t\pm\tau),a)$ or if the relation (4.6) is not satisfied.

(d) $t\in[t_i^--\tau,t_i^-+\tau)$. Then $(t-\tau,t+\tau)\cap I_i=(t-\tau,t_i^-]$ and the expression for $g_i(\mathbf{r},t)$ is identical with (4.16), except the upper integration limit is t_i^-. In the same way as for **(b)** it follows that $g_i(\mathbf{r},t)$ is not differentiable if $\mathbf{r}\in\partial S(\mathbf{r}_i(t-\tau),a)$ or if $\mathbf{r}\in\partial S(\mathbf{r}_i(t_i^-),a)$ or if (4.6) is not satisfied.

(e) $t\geq t_i^-+\tau$. Then $(t-\tau,t+\tau)\cap I_i=\emptyset$ and $g_i(\mathbf{r},t)=0$.

Uniting these sets and taking into account that $t\in(\tau,T-\tau)$ we obtain the set where the function g_i is not differentiable with respect to $\mathbf{r}$

$$\begin{aligned}\Omega_i''=\ &\{(\mathbf{r},t)\mid\quad t\in(t_i^+-\tau,t_i^++\tau]\cap(\tau,T-\tau)\ \text{ and }\ \mathbf{r}\in\partial S(\mathbf{r}_i(t_i^+),a)\}\cup\\ &\{(\mathbf{r},t)\mid\quad t\in[t_i^--\tau,t_i^-+\tau)\cap(\tau,T-\tau)\ \text{ and }\ \mathbf{r}\in\partial S(\mathbf{r}_i(t_i^-),a)\}\cup\\ &\{(\mathbf{r},t)\mid\ t\in(t_i^++\tau,t_i^-+\tau)\cap(\tau,T-\tau)\ \text{ and }\ \mathbf{r}\in\partial S(\mathbf{r}_i(t-\tau),a)\}\cup\\ &\{(\mathbf{r},t)\mid\ t\in(t_i^+-\tau,t_i^--\tau)\cap(\tau,T-\tau)\ \text{ and }\ \mathbf{r}\in\partial S(\mathbf{r}_i(t+\tau),a)\}\cup\\ &\{(\mathbf{r},t)\mid\quad t\in(\tau,T-\tau),\ \text{ exist }\ t'\in(t-\tau,t+\tau)\cap I_i\ \text{ such that}\\ &\qquad\mathbf{r}\in\partial S(\mathbf{r}_i(t'),a)\ \text{ and }\ (\mathbf{r}_i(t')-\mathbf{r})\cdot\boldsymbol{\xi}_i(t')=0\}.\end{aligned}\qquad(4.17)$$

In the same way one can verify that Ω_i'' has the same form for $t_i^--t_i^+\leq 2\tau$. The set Ω_i'' has null Lebesgue measure in $\mathbf{R}^3\times(\tau,T-\tau)$.

Only the terms in (4.15) which contain u in the integration interval have a nonvanishing contribution to the derivative of g_i with respect to x_α. Using (4.8) and taking into account that the sign of the terms in (4.15) coincides

with the sign of the expression -$(\mathbf{r}_i(u)-\mathbf{r})\cdot\boldsymbol{\xi}_i(u)$ which is proportional with the normal component of the velocity of the i-th particle, we obtain

$$\partial_\alpha g_i(\mathbf{r},t) \;=\; \sum_{u\in U_i}\varphi_i(u)\,\frac{x_{\alpha i}(u)-x_\alpha}{\mid(\mathbf{r}_i(u)-\mathbf{r})\cdot\boldsymbol{\xi}_i(u)\mid}, \tag{4.18}$$

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

Using the definition (4.5) and the relations (4.13), (4.14), (4.17), and (4.18) it follows the a.e. continuity of the partial derivatives of $\langle\varphi\rangle$, given by

$$\partial_t\langle\varphi\rangle(\mathbf{r},t) \;=\; \frac{1}{2\tau\mathcal{V}}\sum_{i=1}^{N}[G_i(\mathbf{r},t+\tau)\;-\;G_i(\mathbf{r},t-\tau)] \tag{4.19}$$

for $(\mathbf{r},t)\in\mathbf{R}^3\times(\tau,T-\tau)\backslash\cup_{i=1}^N\Omega_i'$, and

$$\partial_\alpha\langle\varphi\rangle(\mathbf{r},t) \;=\; \frac{1}{2\tau\mathcal{V}}\sum_{i=1}^{N}\sum_{u\in U_i}\varphi_i(u)\,\frac{x_{\alpha i}(u)-x_\alpha}{\mid(\mathbf{r}_i(u)-\mathbf{r})\cdot\boldsymbol{\xi}_i(u)\mid} \tag{4.20}$$

for $(\mathbf{r},t)\in\mathbf{R}^3\times(\tau,T-\tau)\backslash\cup_{i=1}^N\Omega_i''$.

The coarse-grained average $\langle\varphi\rangle$ defined by (4.5) is a linear superposition of the contributions of each individual particle. The average $\langle\varphi\rangle$ is meaningful even for a single particle. In order to intuit the way in which the function $\varphi_i(t)$ is averaged, we consider the case of a particle in a one-dimensional uniform straight motion. The sphere $S(\mathbf{r},a)$ is reduced to an interval $(x-a,x+a)\subset\mathbf{R}$. The particle position is given by the function

$$x_1(t)=\begin{cases} t & \text{if} \quad t\in[t^+,t^-]=I_1\\ 0 & \text{if} \quad t\notin I_1\end{cases} \tag{4.21}$$

where, as discussed in the Chapter 2, a zero coordinate for $t\notin I_1$ is formally assigned to the particle i. In fact the particle does not exist for $t\notin I_1$ and this is taken into account in (4.5) by cancelling the physical quantity φ_i which is averaged. We have chosen (4.21) such that the particle velocity should be equal to unity. In addition the moments t^+ when the particle appears and t^- when it disappears satisfy the inequalities $t^+>\tau$, $t^-<T-\tau$ and $t^--t^+>2\tau$. The averaging parameters a and τ satisfy the relation $\tau<a$. We have chosen the values of t^+, t^-, τ, and a such that they should satisfy these relations only in order to obtain a more intuitive representation.

We calculate the coarse-grained average $\langle\varphi\rangle$ of the function

$$\varphi_1(t)=\begin{cases} 1 & \text{if} \quad t\in I_1\\ 0 & \text{if} \quad t\notin I_1\end{cases} \tag{4.22}$$

and we obtain the discrete analogue of the particles number concentration which we denote by $\langle 1\rangle$. Taking into account that the volume of the sphere $S(\mathbf{r}, a)$ is replaced by the length $2a$ of the spatial interval $(x-a, x+a)$ and that $N = 1$, the relation (4.5) becomes

$$\langle 1\rangle(x,t) \;=\; \frac{1}{4\tau a}\int_{t-\tau}^{t+\tau} \varphi_1(t')\, H^+(a^2-(x_1(t')-x)^2)\, dt'. \tag{4.23}$$

The relation (4.23) takes different forms for (x,t) situated into different regions of the definition domain $\mathbf{R}\times(\tau, T-\tau)$. From (4.21) and (4.22) it follows that for given x the integrand from (4.21) is nonvanishing if $t' \in [t^+, t^-]\cap(x-a, x+a)$. Taking into account the integration limits as well it follows that the integral in (4.21) is equal to the length of the projection on the Ot axis of the interval $[t^+, t^-]\cap(x-a, x+a)\cap(t-\tau, t+\tau)$. Since we have chosen $t^- - t^+ > 2\tau$, for t we consider separately the five variation intervals considered in the proof of the derivative $\partial_\alpha g_i$ continuity.

(a) $t \in (\tau, t^+ - \tau]$. Then $(t-\tau, t+\tau)\cap[t^+, t^-] = \varnothing$ and we have

$$\langle 1\rangle = \quad 0 \quad \text{for} \quad x \in \mathbf{R}.$$

(b) $t \in (t^+ - \tau, t^+ + \tau]$. Then $(t-\tau, t+\tau)\cap[t^+, t^-] = [t^+, t+\tau)$ and because $\tau < a$ the intersection with the interval $(x-a, x+a)$ takes the following values

$$\begin{array}{lll}
\langle 1\rangle = & 0 & \text{for} \quad x \le t^+ - a \\
\langle 1\rangle = & \frac{1}{4\tau a}(x+a-t^+) & \text{for} \quad x \in (t^+ - a, t+\tau-a] \\
\langle 1\rangle = & \frac{1}{4\tau a}(t+\tau-t^+) & \text{for} \quad x \in (t+\tau-a, t^+ + a] \\
\langle 1\rangle = & \frac{1}{4\tau a}(t+\tau-x+a) & \text{for} \quad x \in (t^+ + a, t+\tau+a) \\
\langle 1\rangle = & 0 & \text{for} \quad x \ge t+\tau+a
\end{array}$$

(c) $t \in (t^+ + \tau, t^- - \tau]$. Then $(t-\tau, t+\tau)\cap[t^+, t^-] = [t^+, t+\tau)$ and we have

$$\begin{array}{lll}
\langle 1\rangle = & 0 & \text{for} \quad x \le t-\tau-a \\
\langle 1\rangle = & \frac{1}{4\tau a}(x+a-t+\tau) & \text{for} \quad x \in (t-\tau-a, t+\tau-a] \\
\langle 1\rangle = & \frac{1}{2a} & \text{for} \quad x \in (t+\tau-a, t-\tau+a] \\
\langle 1\rangle = & \frac{1}{4\tau a}(t+\tau-x+a) & \text{for} \quad x \in (t-\tau+a, t+\tau+a) \\
\langle 1\rangle = & 0 & \text{for} \quad x \ge t+\tau+a
\end{array}$$

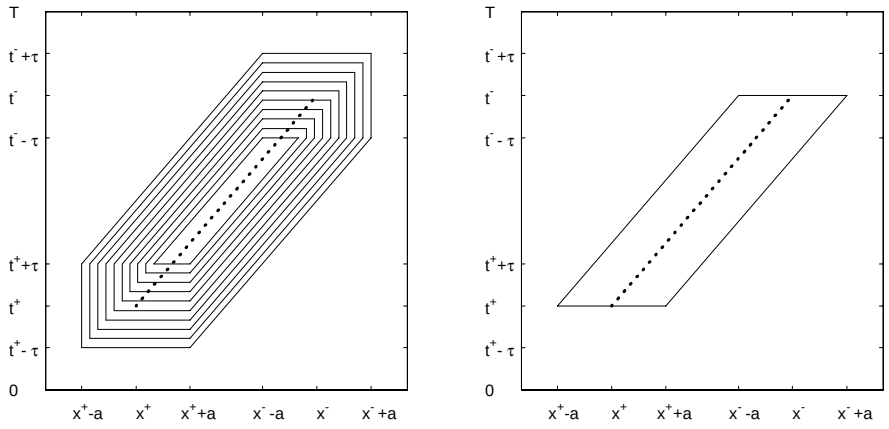

Figure 4.1: The contours of the space-time coarse-grained average and of the spatial average corresponding to the concentration of a single particle in uniform straight motion with unity velocity.

(d) $t \in [t^- - \tau, t^- + \tau)$. Then $(t-\tau, t+\tau) \cap [t^+, t^-] = [t^+, t+\tau)$ and we have

$$\begin{array}{lll} \langle 1 \rangle = & 0 & \text{for} \quad x \leq t - \tau - a \\ \langle 1 \rangle = & \frac{1}{4\tau a}(x + a - t + \tau) & \text{for} \quad x \in (t - \tau - a, t^- - a] \\ \langle 1 \rangle = & \frac{1}{4\tau a}(t^- - t + \tau) & \text{for} \quad x \in (t^- - a, t - \tau + a] \\ \langle 1 \rangle = & \frac{1}{4\tau a}(t^- - x + a) & \text{for} \quad x \in (t - \tau + a, t^- + a) \\ \langle 1 \rangle = & 0 & \text{for} \quad x \geq t^- + a \end{array}$$

(e) $t \geq t^+ - \tau$. Then $(t-\tau, t+\tau) \cap [t^+, t^-] = \varnothing$ and we have

$$\langle 1 \rangle = \quad 0 \quad \text{for} \quad x \in \mathbf{R}.$$

In figure 4.1 we present the coarse-grained average $\langle 1 \rangle$ by means of the contour on which it has the same value. The dotted straight segment represents the particle motion. One can notice that $\langle 1 \rangle$ is continuous, but the first order partial derivatives have discontinuities over a null measure set. It is easy to verify that this set coincides with (4.14) and (4.17). In the regions without discontinuities $\langle 1 \rangle$ is linear in x and t. Simple expressions have been obtained since the particle motion has a very simple form.

In order to emphasize the importance of the time integration in the coarse-grained average definition (4.5), in figure 4.1 we also represented the result obtained only by the space average in (4.5). This comparison is equivalent to that made in the previous section between the formulas (4.1) and (4.3). The difference consists in the fact that there the particles are permanent, whereas

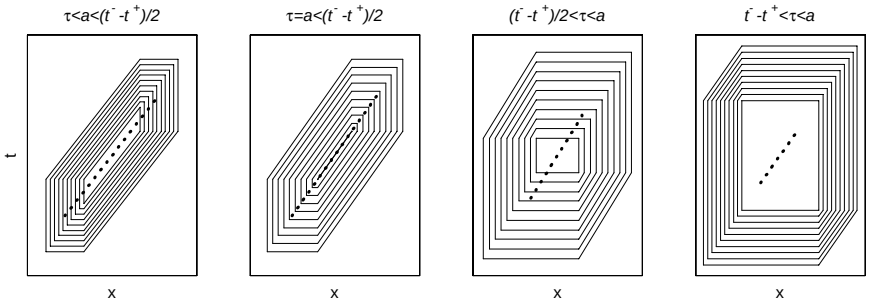

Figure 4.2: The contours of the space-time coarse-grained average and of the spatial average corresponding to the concentration of a single particle in uniform straight motion with unity velocity for different spatial and temporal scales.

now we have a particle which appears and disappears within the time interval $[0, T]$. One notices that by averaging only over space it results a constant value $1/(2a)$ in the parallelogram built on the straight line segment describing the particle motion. This function has a.e. null derivatives. Introducing the time averaging the central region, where $\langle 1 \rangle$ has the value $1/(2a)$, is preserved but the variation from this value to zero in the rest of plan (x, t) is linear, not discontinuous.

If the relations between τ, t^+, and t^- have another form, then it is possible that the region in which $\langle 1 \rangle$ is equal with $1/(2a)$ disappears. In figure 4.2 we have represented the contours of $\langle 1 \rangle$ for other relations between the space and time scales. An interesting case for the discussions in Chapter 6 appears when the averaging interval is very large, so that $(t^+, t^-) \subset (t - \tau,\, t + \tau)$ for any $t \in (t^+, t^-)$. This situation can occur if $t^+ > \tau$, $t^- < T - \tau$ and $2\tau > t^- - t^+$. Then if $t \in (t^+, t^-)$, the integration limits in (4.23) are replaced by t^+ and t^- and the coarse-grained average $\langle 1 \rangle$ does not depend any more on t.

4.3 Balance equations for coarse-grained averages

The coarse-grained average defined in the previous section is not only a.e. of class $\mathbf{C}^1$, but satisfies certain relations having the same form as the balance equations (1.1). We prove that at a point $(r, t) \in R^3 \times (\tau, T - \tau)$ where the derivatives (4.19) and (4.20) exist, the function $\langle \varphi \rangle$ defined by (4.5) satisfies the relation

$$\partial_t \langle \varphi \rangle + \nabla \cdot \langle \varphi \boldsymbol{\xi} \rangle = \langle \dot{\varphi} \rangle + \langle \partial_t \varphi \rangle_g, \tag{4.24}$$

where $\langle \partial_t \varphi \rangle_g$ is a term related to the generation and annihilation of the particles.

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 ([34], p. 331). We apply this theorem to G_i given by (4.12) considered as a function of t. 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 (4.19) it follows that $\partial_t \langle \varphi \rangle$ can also be written as a two term sum

$$\partial_t \langle \varphi \rangle \;=\; (\partial_t \langle \varphi \rangle)' \;+\; (\partial_t \langle \varphi \rangle)''. \tag{4.25}$$

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

$$G_i'(\mathbf{r}, t+\tau) - G_i'(\mathbf{r}, t-\tau) \;=\; \int_{t-\tau}^{t+\tau} \dot{\varphi}_i(t')\, H^+(a^2 - (\mathbf{r}_i(t') - \mathbf{r})^2)\, dt'. \tag{4.26}$$

Dividing (4.26) by $2\tau\mathcal{V}$, summing up with respect to i, and taking into account (4.12), (4.19) and (4.5), we obtain

$$(\partial_t \langle \varphi \rangle)' \;=\; \langle \dot{\varphi} \rangle. \tag{4.27}$$

Thus the absolutely continuous part of the derivative $\partial_t \langle \varphi \rangle$ is given by the continuous time variation of the microscopic quantities φ_i.

From (4.19), the discontinuous part of $\partial_t \langle \varphi \rangle$ can be written as

$$(\partial_t \langle \varphi \rangle)''(\mathbf{r}, t) \;=\; \frac{1}{2\tau\mathcal{V}} \sum_{i=1}^{N} [G_i''(\mathbf{r}, t+\tau) \;-\; G_i''(\mathbf{r}, t-\tau)]. \tag{4.28}$$

It contains the discontinuous variations of G_i during the temporal interval $[t-\tau, t+\tau]$. As proved in the preceding section, $\partial_t \langle \varphi \rangle$ exists if G_i is not discontinuous at $t+\tau$ and $t-\tau$ (see relation (4.14)), therefore we consider only the jumps occurring at the interior points of $[t-\tau, t+\tau]$, i.e., in $(t-\tau, t+\tau)$. From (4.12) it follows that such a variation can take place if the particle is generated inside the sphere $S(\mathbf{r}, a)$ during the temporal interval $(t-\tau, t+\tau)$. Hence the jump of G_i is equal to

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

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

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

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

$$G_i''(\mathbf{r}, t+\tau) \; - \; G_i''(\mathbf{r}, t-\tau) \; = \; \Delta^+ G_i \; + \; \Delta^- G_i \; + \; \sum_{u \in W_i'} \varphi_i(u) \; - \; \sum_{u \in W_i''} \varphi_i(u), \tag{4.29}$$

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 $S(\mathbf{r}, a)$ and it is given by the sign of the expression $-(\mathbf{r}_i(u) - \mathbf{r}) \cdot \boldsymbol{\xi}_i(u)$ which is proportional to the interior normal component of $\boldsymbol{\xi}_i$ to the surface of $S(\mathbf{r}, a)$ at the time u. If we denote $U_i = W_i' \cup W_i''$, we may use a single sum in (4.29). Replacing (4.29) in (4.28) we obtain

$$(\partial_t \langle \varphi \rangle)'' \; = \; \langle \partial_t \varphi \rangle_g \; - \; \frac{1}{2\tau \mathcal{V}} \sum_{i=1}^{N} \sum_{u \in U_i} \varphi_i(u) \, \frac{(\mathbf{r}_i(u) - \mathbf{r}) \cdot \boldsymbol{\xi}_i(u)}{\mid (\mathbf{r}_i(u) - \mathbf{r}) \cdot \boldsymbol{\xi}_i(u) \mid}, \tag{4.30}$$

where

$$\langle \partial_t \varphi \rangle_g \; = \; \frac{1}{2\tau \mathcal{V}} \sum_{i=1}^{N} (\Delta^+ G_i \; + \; \Delta^- G_i). \tag{4.31}$$

Since $\varphi_i(t)$ and $\xi_{\alpha i}(t)$ are analytic functions with respect to time, then their product is also analytic and the relation (4.30) can be written as

$$(\partial_t \langle \varphi \rangle)'' \; = \; -\nabla \cdot \langle \varphi \boldsymbol{\xi} \rangle \; + \; \langle \partial_t \varphi \rangle_g. \tag{4.32}$$

The physical quantity $\varphi_i \boldsymbol{\xi}_i$ represents the transport of φ by the particle i with the velocity $\boldsymbol{\xi}_i$ and $\langle \varphi \boldsymbol{\xi} \rangle$ is the mean flux of φ. The relation (4.24) results from (4.25), (4.27) and (4.32).

In contrast to the balance equation (1.1), the relation (4.24) does not contain a term describing the transport due to the mean motion of the particles and implicitly a quantity equivalent to the mean baricentric velocity $\mathbf{u}$ (definition (3.10)). The velocity is not a volume density, but an average quantity. To define a discrete analogue of a mean quantity, we have to divide $\langle \varphi \rangle$ by the mass of the particles contributing to the value of $\langle \varphi \rangle$. Let $\langle m \rangle$ be the coarse-grained average (4.5) corresponding to the particles mass $\varphi_i(t) = m_i$ for all $t \in I_i$ and $i \leq N$. Since $\langle m \rangle$ characterizes the mean mass of the particles per unit volume, it represents the discrete analogue of the mass density. The discrete mean of φ is defined as

$$\overline{\varphi}(\mathbf{r}, t) \; = \begin{cases} \langle \varphi \rangle(\mathbf{r}, t) / \langle m \rangle(\mathbf{r}, t) & \text{if} \quad \langle m \rangle(\mathbf{r}, t) \neq 0 \\ 0 & \text{if} \quad \langle m \rangle(\mathbf{r}, t) = 0 \end{cases} . \tag{4.33}$$

It is easy to show that the mean (4.33) has the properties $\overline{\overline{\varphi}} = \overline{\varphi}$, $\overline{\varphi_1 + \varphi_2} = \overline{\varphi_1} + \overline{\varphi_2}$ and $\overline{\lambda\varphi} = \lambda\overline{\varphi}$, where λ is a real function of $\mathbf{r}$ and t.

Analogously to (3.10), the mean motion of the particles is defined by the discrete average (4.33) of the momentum $\overline{\mathbf{p}}$ with the components $\overline{p}_\alpha$. To introduce the mean velocity in (4.24), we write

$$\langle\varphi\xi_\alpha\rangle \;=\; \langle\varphi[\overline{p}_\alpha + (\xi_\alpha - \overline{p}_\alpha)]\rangle \;=\; \langle\varphi\rangle\overline{p}_\alpha \;+\; (\mathbf{\Phi}'_\varphi)_\alpha,$$

where the vector $\mathbf{\Phi}'_\varphi$ is the discrete analogue of the kinetic part of the flux density of φ and its components are

$$(\mathbf{\Phi}'_\varphi)_\alpha \;= \langle\varphi(\xi_\alpha - \overline{\xi}_\alpha)\rangle \;. \tag{4.34}$$

Then (4.24) becomes

$$\partial_t\langle\varphi\rangle \;+\; \nabla\cdot(\langle\varphi\rangle\overline{\mathbf{p}}) \;+\; \nabla\cdot\mathbf{\Phi}'_\varphi \;=\; \langle\dot{\varphi}\rangle \;+\; \langle\partial_t\varphi\rangle_g. \tag{4.35}$$

This is the discrete analogue of the balance equation (1.1).

As a simple application of these results we write (4.35) for mass, momentum, and kinetic energy in the case of the Hamiltonian corpuscular system described at the end of the Chapter 2. Thus we obtain the discrete analogue of the balance equations derived in chapter 3 by the methods in statistical mechanics. The analogy is not valid for the interaction potential energy and therefore neither for the total energy since the statistical averaging (3.4) is punctual whereas the coarse-grained average (4.5) refers to the finite volume of the sphere $S(\mathbf{r}, t)$. In the next section this problem is solved by the statistical averaging of the discrete analogue of the balance equation (4.24).

The abstract particles defined in chapter 2 with which we have worked till now in this chapter become real particles with the mass m_i satisfying the classical mechanics laws Since the particles are not generated or destroyed we have $I_i = I$ for any $i \leq N$ and the generation term (4.31) vanishes in all the balance equations. For mass we choose $\varphi_i(t) = m_i$ for any $i \leq N$. Then $\langle\varphi\rangle = \langle m\rangle$ is the discrete analogue of the mass density. Instead of (4.35) we can use directly (4.24) and from the definition (4.33) for the mean velocity we obtain

$$\partial_t\langle m\rangle \;+\; \nabla\cdot(\langle m\rangle\overline{\mathbf{p}}) \;=\; 0, \tag{4.36}$$

that is the discrete analogue of the continuity equation (3.14).

In order to obtain the discrete analogue of the diffusion equation (1.5) we have to consider that the ensemble of the N particles is formed from several components, each of them having the same type of particles. We denote by $i \leq N' < N$ the particles of the mixture component for which we write the diffusion equation. Considering the formula (4.3), it follows that to obtain

the discrete analogue of the concentration of the particles $i \leq N'$ we have to apply the coarse-grained average (4.5) for $\varphi_i(t) = 1$ if $i \leq N'$ and $\varphi_i(t) = 0$ if $N' < i \leq N$. We denote this coarse-grained by $\langle 1' \rangle$. Since $\dot{\varphi}_i(t) = 0$, the relation (4.35) becomes

$$\partial_t \langle 1' \rangle + \nabla \cdot (\langle 1' \rangle \bar{\mathbf{p}}) + \nabla \cdot \mathbf{\Phi}'_{1'} = 0, \tag{4.37}$$

that is the discrete analogue of the equation (1.5). From (4.34) one notices that the discrete analogue $\mathbf{\Phi}'_{1'}$ of the density of the particles flux $\mathbf{j}$ from (1.5) is the density of the mean relative velocity of the particles $i \leq N'$ with respect to the baricentric mean velocity $\bar{\mathbf{p}}$.

For the component α of the momentum we have $\varphi_i = p_{\alpha i} = m_i \xi_{\alpha i}$ and $\langle p_\alpha \rangle = \langle m \rangle \overline{p}_\alpha$. The time derivative $\dot{\varphi}_i$ is the component α of the force $\mathbf{F}_i$ acting on the particle i. Then the relation (4.35) takes the form

$$\partial_t(\langle m \rangle \overline{p}_\alpha) + \sum_{\beta=1}^{3} \partial_\beta(\langle m \rangle \overline{p}_\alpha \overline{p}_\beta) - \sum_{\beta=1}^{3} \partial_\beta T'_{\alpha\beta} = \langle F_\alpha \rangle, \tag{4.38}$$

where from (4.34) it follows that

$$T'_{\alpha\beta} = -\langle m(\xi_\alpha - \overline{p}_\alpha)(\xi_\beta - \overline{p}_\beta) \rangle \tag{4.39}$$

is a symmetric tensor corresponding to the kinetic part $\sigma'_{\alpha\beta}$ of the stress tensor (3.19). One notices that the relation (4.39) is the discrete analogue of the balance equation for momentum (3.18).

For the kinetic energy of the particles $\varphi_i = \frac{1}{2} m_i \boldsymbol{\xi}_i^2$, we have

$$\langle \varphi \rangle = \frac{1}{2} \langle m \rangle \bar{\mathbf{p}}^2 + \frac{1}{2} \langle m \overline{\mathbf{p}} \cdot (\boldsymbol{\xi} - \overline{\mathbf{p}}) \rangle + \frac{1}{2} \langle m (\boldsymbol{\xi} - \overline{\mathbf{p}})^2 \rangle.$$

The second term vanishes because $\langle \overline{\mathbf{p}} \cdot (\boldsymbol{\xi} - \overline{\mathbf{p}}) \rangle = \overline{\mathbf{p}} \cdot \langle \boldsymbol{\xi} - \overline{\mathbf{p}} \rangle = 0$. The last term is the discrete analogue of the kinetic energy density of the thermic motion ε given by (3.23), since $m(\boldsymbol{\xi}_i - \overline{\mathbf{p}})^2/2$ represents the kinetic energy of the relative motion of the particle i with respect to the mean motion of the particles in the sphere $S(\mathbf{r}, a)$ over the interval $(t - \tau, t + \tau)$. We denote this term by

$$\langle \varepsilon' \rangle = \frac{1}{2} \langle m (\boldsymbol{\xi} - \overline{\mathbf{p}})^2 \rangle \,. \tag{4.40}$$

Similarly we show that

$$(\mathbf{\Phi}_\varphi)_\alpha = \frac{1}{2} \langle m \, \boldsymbol{\xi}^2 (\boldsymbol{\xi} - \overline{\mathbf{p}}) \rangle = \frac{1}{2} \sum_{\beta=1}^{3} \bar{p}_\beta T'_{\alpha\beta} + (\mathbf{\Phi}'_\varepsilon)_\alpha$$

where the kinetic energy flux of the relative motion of the particles is defined by

$$\mathbf{\Phi}'_{\varepsilon} = \frac{1}{2}\langle m(\boldsymbol{\xi} - \overline{\mathbf{p}})^2(\boldsymbol{\xi} - \overline{\mathbf{p}})\rangle \tag{4.41}$$

and it is the discrete analogue of the kinetic part of the heat flux density $\mathbf{q}'$ (3.26). Taking into account that $\dot{\varphi}_i = m\boldsymbol{\xi}_i \cdot \dot{\boldsymbol{\xi}}_i = \boldsymbol{\xi}_i \cdot \mathbf{F}_i$, the relation (4.35) becomes

$$\partial_t \left(\frac{1}{2}\langle m\rangle\overline{\mathbf{p}}^2 + \langle\varepsilon'\rangle\right) + \nabla\cdot\left[\left(\frac{1}{2}\langle m\rangle\overline{\mathbf{p}}^2 + \langle\varepsilon'\rangle\right)\overline{\mathbf{p}}\right] + \nabla\cdot\mathbf{\Phi}'_{\varepsilon} + \frac{1}{2}\sum_{\alpha,\beta=1}^{3}\partial_\alpha(\bar{p}_\beta T'_{\alpha\beta}) = \langle\boldsymbol{\xi}\cdot\mathbf{F}\rangle \tag{4.42}$$

which represents the discrete analogue of the balance equation for kinetic energy (3.25).

We emphasize that the relations (4.36), (4.37), (4.38), and (4.42) are not balance equations, but identities of the same form of the corresponding balance equations (3.14), (3.16), (3.18), and (3.25). One can say the same on the relations for an arbitrary physical quantity (4.24) and (4.35) with respect to the balance equations (3.12) and (3.13). The relations derived in this chapter preserve, at the set points (4.14) and (4.17), the discontinuities of the microscopic discrete description. The transformation of the function $\langle\varphi\rangle$ into a continuous field and of the relation (4.35) into a balance equation is performed through an averaging that should smooth the implied functions. The methods that can do this averaging are discussed in the next section.

4.4 The statistical averaging of the coarse-grained averages

The relations (4.24) and (4.35) satisfied by the coarse-grained average (4.5) have the form of the balance equations (1.1), but they do not have the necessary smoothness. What is important is that they have been derived under very general conditions, their existence being proved for any physical system with corpuscular structure, regardless of the laws governing the motion of the constituent particles. The smoothness necessary to the continuous fields can be obtained as in Chapter 3 assuming that there exists a probability density in the phase space. In Chapter 3 we have assumed that the probability density satisfies the Liouville equation (3.2). Now we can generalize this result for the case when there exists a probability density without the need to know if its evolution satisfies any equation in the phase space. This is possible since (4.24) and (4.35) have already the form of the balance equations.

The coarse-grained average (4.5) is equal to the linear superposition of all the particles contributions to all the moments within the interval $(t-\tau, t+\tau)$. Therefore the statistical average (3.3) of the coarse-grained average (4.5) is obtained by summing up the statistical averages of the elementary contributions given by the function $G_i(\mathbf{r},t)$ from (4.12), that is

$$\overline{\langle\varphi\rangle}(\mathbf{r},t)=\frac{1}{2\tau\mathcal{V}}\sum_{i=1}^{N}\int_{t-\tau}^{t+\tau}\bar{G}_i(\mathbf{r},t')\,dt'\,.$$

If we denote by f_i the function from the phase space attached to the physical quantity φ_i by means of a relation of the type (2.2)

$$\varphi_i(t)=f_i(\mathbf{R}(t),\mathbf{P}(t),t)\,, \tag{4.43}$$

then we have

$$\begin{aligned}\bar{G}_i(\mathbf{r},t) &= \int\int f_i(\mathbf{R},\mathbf{P},t)\,P(\mathbf{R},\mathbf{P},t)\,H^+(a^2-(\mathbf{r}_i-\mathbf{r})^2)\,d\mathbf{R}\,d\mathbf{P}\\ &= \int_{S(\mathbf{r},a)}d\mathbf{r}'\int\int f_i(\mathbf{R},\mathbf{P},t)\,\delta(\mathbf{r}_i-\mathbf{r}')\,P(\mathbf{R},\mathbf{P},t)\,d\mathbf{R}\,d\mathbf{P}\end{aligned} \tag{4.44}$$

Using the definition (3.4) of the average volume density it results the relation

$$\overline{\langle\varphi\rangle}(\mathbf{r},t)=\frac{1}{2\tau\mathcal{V}}\int_{t-\tau}^{t+\tau}\int_{S(\mathbf{r},a)}D_f(\mathbf{r}',t')\,d\mathbf{r}'dt', \tag{4.45}$$

which relates the usual statistical approach from chapter 3 to that presented in this chapter.

Using (4.44) in the statistical averaging (3.3) of the time derivative (4.19) we have

$$\overline{\partial_t\langle\varphi\rangle}(\mathbf{r},t)=\frac{1}{2\tau\mathcal{V}}\int_{S(\mathbf{r},a)}[D_f(\mathbf{r}',t+\tau)-D_f(\mathbf{r}',t-\tau)]d\mathbf{r}'\,. \tag{4.46}$$

Since

$$\partial_\alpha\langle\varphi\rangle(\mathbf{r},t)=\frac{1}{2\tau\mathcal{V}}\sum_{i=1}^{N}\int_{t-\tau}^{t+\tau}\partial_\alpha\bar{G}_i(\mathbf{r},t')\,dt'$$

from (4.44) it follows

$$\overline{\partial_\alpha\langle\varphi\rangle}(\mathbf{r},t)=\frac{1}{2\tau\mathcal{V}}\int_{t-\tau}^{t+\tau}\partial_\alpha\int_{S(\mathbf{r},a)}D_f(\mathbf{r}',t')d\mathbf{r}'dt'.$$

Making the change of variable $\mathbf{r}' = \mathbf{r}'' + \mathbf{r}$ we obtain

$$\partial_\alpha \int_{S(\mathbf{r},a)} D_f(\mathbf{r}', t')d\mathbf{r}' = \int_{S(0,a)} \partial_\alpha D_f(\mathbf{r}'' + \mathbf{r}, t')\, d\mathbf{r}'' .$$

Since $\partial_\alpha D_f(\mathbf{r}'' + \mathbf{r}, t') = \partial''_\alpha D_f(\mathbf{r}'' + \mathbf{r}, t')$ and making the inverse change of variable $\mathbf{r}'' = \mathbf{r}' + \mathbf{r}$, it follows

$$\overline{\partial_\alpha \langle\varphi\rangle}(\mathbf{r}, t) = \frac{1}{2\tau\mathcal{V}} \int_{t-\tau}^{t+\tau} \int_{S(\mathbf{r},a)} \partial'_\alpha D_f(\mathbf{r}', t')d\mathbf{r}'dt'. \tag{4.47}$$

In the relations (4.45)-(4.47) we have obtained the statistical average (3.3) of the discrete analogue of the balance equation (4.24). For the Hamiltonian systems the term due to the particles generation is null and taking into account that the sphere $S(\mathbf{r}, a)$ is arbitrary it follows

$$\frac{1}{2\tau}[D_f(\mathbf{r}', t+\tau) - D_f(\mathbf{r}', t-\tau)] + \frac{1}{2\tau} \int_{t-\tau}^{t+\tau} \nabla \cdot D_{f\boldsymbol{\xi}}(\mathbf{r}, t')dt' = \frac{1}{2\tau} \int_{t-\tau}^{t+\tau} D_{\hat{f}}(\mathbf{r}, t')dt'.$$

For $\tau \to 0$ it is possible to apply the mean value theorem and we obtain the balance equation (3.12)

$$\partial_t D_f + \nabla \cdot D_{f\boldsymbol{\xi}} = D_{\hat{f}} \ . \tag{4.48}$$

As noticed, the difference is that now the derivation has been performed without any hypotheses on the evolution equation satisfied by the probability distribution $P(\mathbf{R}, \mathbf{P}, t)$. We have used only the existence of $P(\mathbf{R}, \mathbf{P}, t)$.

In the previous derivation of the general balance equation (4.48) the form of the balance equations existed already in the relations (4.24) and (4.35). The existence of the balance equations can be justified using these relations and the local equilibrium principle instead of the probability distribution existence. If the parameters a and τ are chosen such that within the time interval $(t - \tau, t + \tau)$ the particles in the sphere $S(\mathbf{r}, a)$ should form a near the equilibrium thermodynamic system, then the definition (4.5) supplies ordinary continuous macroscopic fields and the relations (4.24) and (4.35) become balance equations. The smoothness specific to the macroscopic fields is obtained assuming that the particles locally behave as a system in thermodynamic equilibrium. The local equilibrium principle can be applied not only for the most general form of the corpuscular systems but for special cases too. For example, for the Hamiltonian corpuscular system in chapter 2, the relations (4.36), (4.37), (4.38), and (4.42) are transformed into usual balance equations (3.14), (3.16), (3.21), and (3.25). This is a verification that in the case when the statistical mechanics allows to obtain the balance equations, these coincide with those derived by means of the coarse-grained averages.