Chapter 2

Corpuscular systems

The usual method to derive the macroscopic description by means of the continuous field for a physical corpuscular system starting from its discontinuous microscopic structure is that initiated by Boltzmann in classical statistical mechanics [1], [4], [12], [21]. This method relies on the evolution equation of the probability density in the phase space of the ensemble of all the microscopic components of the physical system (Liouville equation). Using the BBGKY chain, i.e., a sequence of projections on the multiparticle spaces, the Boltzmann equation is obtained in the one-particle space. For the collisional invariants (mass, moment and energy) the usual hydrodynamic equations result by an averaging over the moments. Even for the simple case of the ideal gas, because of the mathematical difficulties, the derivation of the balance equations and constitutive relations is possible only using several hypotheses, approximations, and simplifications [11]. So far, these results have been extended to hard sphere fluids, also a very idealized molecular model [13].

In the nonequilibrium statistical mechanics the Liouville equation plays the same role as the local equilibrium principle in thermodynamics, that is the role of a bridge between the microscopic corpuscular description and the macroscopic continuous description. The Liouville equation combine in its structure both characteristics of the microscopic scale and those of the macroscopic one. Its microscopic nature is obvious since it is defined on the phases space formed by all the possible microscopic states of the corpuscular system and it is a reflection of the Hamiltonian dynamics of the microscopic state. In addition the Liouville equation can be written only if the forces of interaction between the microscopic components are known, i.e., the model of the microscopic structure of the physical system has to be completely described. But the Liouville equation has some characteristics specific to the continuous macroscopic description. First the probability density is a continuous field in the phase space, not in the three-dimensional Euclidian

space. Hence the probability density and its derivatives have the smoothness characteristic to the continuous macroscopic description. Then the Liouville equation has the form specific to balance equations because it represents the local form of the probability conservation in phase space.

An important characteristic of the statistical mechanics method is that both the balance equations and constitutive relations are obtained *simultaneously* by projecting the Liouville equation. However their origin is different. In this work we show that the form of the balance equations can be derived using just the fact that at microscopic level the macroscopic body has a corpuscular structure. More exactly, it is essential that the microscopic particles preserve their identity over a finite time interval within which their motion can be described by piece-wise analytical time functions. Thus the macroscopic conservation laws embodied by the balance equations are the reflection at macroscopic scale of the transport of the microscopic quantities through continuous displacements of the constituent particles. The balance equations describe the mean movement as whole of the microscopic particles.

Unlike the balance equations, the constitutive relations result from the dynamic laws governing the microscopic motion of the constituent particles. In general the derivation of the constitutive relations is particularly difficult and therefore its separation from the balance equation derivation can facilitate the analysis of the macroscopic behavior of the corpuscular systems. An example that we deal with in Chapter 9 is the description of the global evolution of a financial market. The "microscopic" corpuscular structure of this system is formed by individual assets whose price varies according to laws which cannot be given by differential or stochastic equations. However, as for a fluid formed by molecules, we will show that the global evolution of a financial market can be described by balance equations.

In this work we show that the continuous macroscopic description of an arbitrary corpuscular system can be derived in three successive stages [63], [64]. First we prove that for an arbitrary finite number of material points there exists a space-time coarse-grained average satisfying a mathematical relation of the form of a balance equation. These coarse-grained averages have discontinuous first order partial derivatives. They can be defined only for additive physical quantities which can be attributed to the individual microscopic particles. Since the entropy does not satisfy this condition (the entropy characterizes the ensemble of all particles of the thermodynamic system) the balance equation for entropy can not be derived by this method. In the rest there is no restriction on the physical quantities for which the balance equation is derived. So the existence of a relation having the form of a balance equation depends on the existence of a *kinematic description* of the microscopic evolution. The smoothness specific to the continuous macro-

scopic fields is obtained in the second stage if the physical system verifies the local equilibrium assumption or if in the phase space of the ensemble of the microscopic particles there is a smooth probability distribution. In the third stage the information on the microscopic structure is used to derive the constitutive relations. In this way the independence of the balance equations on the microscopic structure is emphasized. The usual statistical approach does not allow the separation of the three stages, all of them being simultaneously implied in the Liouville equation.

Since we need a kinematic microscopic description of the corpuscular system, we use a very general mathematical model for the corpuscular systems [64]. Due to this generality, the results obtained can be particularized for Hamiltonian as well. We study the evolution during the temporal interval $I = [0, T] \subset \mathbf{R}$ of a finite and arbitrary number N of abstract particles. In the following we will explain what we mean by the abstract nature of these particles. The particles can appear and disappear as a consequence of some instantaneous processes. Each particle i $(1 \leq i \leq N)$ has an interval of existence $I_i = [t_i^+, t_i^-] \subset I$ which can differ from I, that is $0 \leq t_i^+ < t_i^- \leq T$. If $I_i = I$, then the particle i exists during the whole interval I. If $I_i \neq I$ for at least one particle, 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 particles at time $t \in I$, we have $n(t) \leq N$ for every $t \in I$. The equality $n(t) = N$ holds only if $I_i = I$ for all $i \leq N$, i.e., if no particle is generated or destroyed over the interval I. We also notice that only one existence interval corresponds to a given particle, that is its disappearance at a given moment excludes the possibility of its reappearance. Even if a particle of the same type reappears subsequently, it is considered as a new particle. The abstract nature of the considered system is also given by the fact that we impose no link between the appearance of some particles and the disappearance of the others. It is obvious that in the case of a particular corpuscular system in which chemical reactions take place, such links exist and they must be explicitly considered.

Arbitrary time functions of abstract nature are associated to each particle, in the sense that they have not a precise physical meaning. For a given corpuscular system, these time functions may represent the mass of particles, their momentum or any other physical quantity but also, for example, the price of an asset. Let $\varphi_i : I \to \mathbf{R}$ be such an arbitrary function characterizing the particle i. If $I_i \neq I$, then we impose that $\varphi_i(t) = 0$ for all $t \in I \setminus I_i$. The extension of the definition domain of the functions φ_i from the interval I_i to the whole interval I the function φ_i taking an arbitrary constant value in the exterior of I_i is a formal method to simplify the averaging formulas in which only the interval I appears and not the intervals I_i. In the interval I_i the

function φ_i may take any real value, including zero. Hence φ_i is discontinuous in t_i^+ and t_i^- if $\varphi_i(t_i^+) \neq 0$ and $\varphi_i(t_i^-) \neq 0$. Similarly, the derivatives of φ_i in t_i^+ and t_i^- may be continuous or discontinuous. We have denoted the physical quantity by φ and not by Ψ as we did in the chapter 1 since there are balance equations for additive physical quantities which can not be attributed to a single molecule or to a limited group of molecules (for example the entropy).

We consider that we have a complete kinematic description of the motion of all particles, i.e., we assume that the position of each particle is given by a mathematical point whose movement is known. So the components $x_{\alpha i} : I \to \mathbf{R}$ $(\alpha = 1, 2, 3)$ of the radius vector $\mathbf{r}_i$ of the mathematical point associated to the particle i are particular cases of time functions φ_i. The kinematic nature of the information from which we begin our approach is very important. We know nothing on the dynamic laws governing the particles motion. If the evolution of the particles ensemble can be modeled, for example, by a system of differential equations, we do not need to know their form. It is sufficient to know that they have a solution which satisfies the conditions claimed for the *existence* of the functions φ_i. But neither the possibility of the modeling of the particles evolution by a dynamic system is necessary. For example, it is questionable if the psychical processes of the traders in a financial market can be mathematically modelled, nevertheless the prices evolution can be described kinematically. So, our kinematic description is also valid for nonmechanical phenomena (for example, for electrical, social, biological, etc. quantities). In this case the quality of kinematic refers to the fact that quantities vary in time, but similarly to the usual mechanic quantities (position, momentum, etc.) it is not necessary to know the laws ruling this variation.

The only condition imposed to the functions φ_i, and consequently to the particles motion is that the restriction $\varphi_i|I_i$ be analytical. Then $\varphi_i|I_i$ has continuous derivatives of any order and the associated Taylor series converges. Under these conditions the velocity of the particles $\boldsymbol{\xi}_i = \dot{\mathbf{r}}_i$ exists and its components $\xi_{\alpha i} : I \to \mathbf{R}$ $(\alpha = 1, 2, 3)$ are particular cases of the functions φ_i. This condition does not significantly restrain the application domain of our method, because the particles can appear and disappear. When a discontinuity occurs in the motion of a particle, then we assume that the old particle disappears and a new one is generated in the same moment, of the same type and with the values of the functions φ_i equal to those after the discontinuity. 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. Hence, any corpuscular physical system whose evolution can be described by piecewise analytical functions belongs to the

type of functions to which the above approach can be applied.

In the following we particularize the abstract discrete system previously defined in the case of the Hamiltonian systems formed by permanent particles as those usually considered in statistical mechanics. For any $i \leq N$, we have $I_i = I$ and the number of particles does not vary in time. The abstract particles become real particles with a constant mass m_i. The laws ruling the motion of the particles ensemble are given by Hamilton's equations [38]. We assume that the particles remain separated, such that the generalized coordinates of the system are given by the particles positions $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$ and by their momentums $\mathbf{P} = (\mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_N)$ with $\mathbf{p}_i = m_i \boldsymbol{\xi}_i$. Then there exists Hamiltonian $H(\mathbf{R}, \mathbf{P}, t)$, defined in the extended phases space $\mathbf{R}^{6N} \times [0, T]$, by means of which the equations of motion read

$$\dot{\mathbf{r}}_i = \frac{\partial H}{\partial \mathbf{p}_i} \ , \ \dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{r}_i}. \tag{2.1}$$

A particular solution of these equations is obtained if the initial conditions $\mathbf{R}_0 = \mathbf{R}(0)$ and $\mathbf{P}_0 = \mathbf{P}(0)$ are specified. We denote it by $\mathbf{R}(t) = \mathbf{R}(\mathbf{R}_0, \mathbf{P}_0, t)$ and $\mathbf{P}(t) = \mathbf{P}(\mathbf{R}_0, \mathbf{P}_0, t)$. This solution provides a kinematic description of the Hamiltonian system evolution of the type discussed previously. If $f = f(\mathbf{R}, \mathbf{P}, t)$ is a function defined in the extended phase space then its evolution in time can be described kinematically by the function

$$\varphi(t) = f(\mathbf{R}(t), \mathbf{P}(t), t). \tag{2.2}$$

When f is a mechanical quantity referring to a single particle (the kinetic energy, angular momentum, etc.), the relation (2.2) represents a time function φ_i of the type previously defined. The notation used in (2.2) is maintained all over the work. The physical quantities whose evolution is known in the phase space of a dynamic system are denoted with Latin letters (more frequently with f). Those for which we have only a kinematic description, without knowing the dynamic system which rules its evolution, are denoted with Greek letters (more frequently with φ). In other words, for quantities of f type we know the generator of the dynamic system, as for quantities φ, we do not know it.