

# Chapter 2

## From the Phase Space to the Boltzmann Equation

In this chapter, we will outline the general mathematical framework concerning the statistical description of a many-particle system in the phase space. We will then restrict our analysis to the single-particle space and will sketch the derivation of the Boltzmann equation, which was originally derived by Ludwig Boltzmann (1872) for a hard-spheres gas by merging mechanical concepts and statistical considerations.

### 2.1 The Phase Space Description

Let us consider a system of  $N$  identical particles, described by the coordinates  $(\mathbf{q}_i, \mathbf{p}_i)$ , with  $i = 1, \dots, N$ , which denote, respectively, the positions and the momenta of the particles. For convenience, we will use the shorthand notation  $(\mathbf{Q}, \mathbf{P})$  to refer to the entire set of coordinates in a compact phase space  $\mathcal{U} \subset \mathbb{R}^{6N}$ . The time evolution of this system is given by a flow  $S^t : \mathcal{U} \rightarrow \mathcal{U}$ , with  $S^t$  denoting a one-parameter group of diffeomorphisms. We focus hereinafter on conservative dynamical systems whose dynamics is dictated by the Hamiltonian  $H(\mathbf{Q}, \mathbf{P})$ , with an interaction term defined by a (smooth) pairwise potential  $\Phi : \mathbb{R}^3 \rightarrow \mathbb{R}$ , depending only on the distance  $|\mathbf{q}_i - \mathbf{q}_j|$  between the  $i$ th and  $j$ th particles. The dynamical systems under consideration are, moreover, equipped with a probability measure  $\mu(d\mathbf{Q}d\mathbf{P})$ , with support on  $\mathcal{U}$ , absolutely continuous with respect to the Lebesgue measure. Hence, we suppose that a phase space density  $F(\mathbf{Q}, \mathbf{P})$ , positive definite and normalized, exists and is such that  $F(\mathbf{Q}, \mathbf{P})d\mathbf{Q}d\mathbf{P}$  represents the probability of finding the system in the phase space element centered at the point  $(\mathbf{Q}, \mathbf{P}) \in \mathcal{U}$ . The trajectory of  $(\mathbf{Q}, \mathbf{P})$  is determined by solving Hamilton's equations

$$\dot{\mathbf{q}}_i(t) = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i(t) = -\frac{\partial H}{\partial \mathbf{q}_i}, \quad (2.1)$$

for each  $i = 1, \dots, N$ .

Let us introduce, then, the phase space functions, also called microscopic dynamical functions,  $a(\mathbf{Q}, \mathbf{P}) : \mathcal{U} \rightarrow \mathbb{R}$ , which, under the evolution in the phase space, are transformed, at time  $t$ , into  $a(\mathbf{Q}, \mathbf{P}, t)$ . It is useful to let the phase functions depend also on a vector-valued parameter  $\mathbf{r}$ , which in the sequel will denote the position vector in the physical space. We restrict ourselves to smooth phase space functions, which form a Lie algebra, given by the Poisson bracket  $\{\cdot, \cdot\}$ , defined as

$$\{a_1, a_2\} = \sum_{i=1}^N \left( \frac{\partial a_1}{\partial \mathbf{q}_i} \frac{\partial a_2}{\partial \mathbf{p}_i} - \frac{\partial a_1}{\partial \mathbf{p}_i} \frac{\partial a_2}{\partial \mathbf{q}_i} \right).$$

From Eq. (2.1), the time evolution equation for  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$  can be written in the form

$$\partial_t a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t) = \{a, H\}, \quad (2.2)$$

where  $\partial_t$  denotes the partial derivative with respect to time. The values of  $(\mathbf{Q}(t), \mathbf{P}(t))$  at time  $t$ , obtained by solving Eq. (2.1) for given initial values  $(\mathbf{Q}, \mathbf{P})$ , are expressed by the following canonical transformations [1]:

$$(\mathbf{Q}(t), \mathbf{P}(t)) = S^t(\mathbf{Q}, \mathbf{P}), \quad \text{with } S^t = e^{\mathcal{L}t}, \quad (2.3)$$

where  $\mathcal{L}[\cdot] = \{\cdot, H\}$  is the *Liouville operator*. The time-evolved phase function  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$  can be computed from Eq. (2.2) and also by exploiting the canonical transformations (2.3). It attains the form

$$a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t) = e^{\mathcal{L}t} a(\mathbf{Q}, \mathbf{P}, \mathbf{r}) = a(e^{\mathcal{L}t}(\mathbf{Q}, \mathbf{P}), \mathbf{r}), \quad (2.4)$$

which holds under the assumption of smoothness of the phase functions  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$ . In other words, under a canonical transformation, a (smooth enough) dynamical function  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r})$  goes over the same function of its time-evolved arguments. At the macroscopic level, the relevant quantities are represented by continuous functions in the physical space–time, which we denote by  $A(\mathbf{r}, t)$ . One of the basic tenets of statistical mechanics claims that for any observable  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$ , there exists a unique macroscopic function  $A(\mathbf{r}, t)$ , given by the *ensemble average* of  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$ , with respect to the density  $F(\mathbf{Q}, \mathbf{P})$ :

$$A(\mathbf{r}, t) = \langle a \rangle = \int a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t) F(\mathbf{Q}, \mathbf{P}) d\mathbf{Q} d\mathbf{P}. \quad (2.5)$$

It is worth remarking that the converse does not hold. There exist, in fact, certain thermal quantities, which typically play an important role in thermodynamics, that do not enjoy a mechanical definition and cannot be defined as shown in Eq. (2.5). For instance, one such quantity is the entropy, which is not a property of a single particle, but rather describes the overall “state of disorder” of the system. In this case,

the corresponding dynamical function  $a(\mathbf{Q}, \mathbf{P}, \mathbf{r}, t)$  is not a given, fixed microscopic dynamical function, but it depends on the probability density  $F(\mathbf{Q}, \mathbf{P})$  [1]. Using Eq. (2.4), we can rewrite Eq. (2.5) as

$$A(\mathbf{r}, t) = \int \left[ e^{\mathcal{L}t} a(\mathbf{Q}, \mathbf{P}, \mathbf{r}) \right] F(\mathbf{Q}, \mathbf{P}) d\mathbf{Q} d\mathbf{P}, \quad (2.6)$$

which therefore expresses the law of motion of a macroscopic quantity as induced by the Hamiltonian dynamics of the corresponding observable in the phase space. Equation (2.6) suggests an analogy with the Heisenberg representation of quantum mechanics: the average is computed by keeping the state of the system fixed and by letting the dynamical phase space variables evolve in time. Conversely, in the Schrödinger-like picture, one may transfer the time dependence from the microscopic dynamical function to the probability density by employing the time-evolved density

$$F(\mathbf{Q}, \mathbf{P}, t) = e^{-\mathcal{L}t} F(\mathbf{Q}, \mathbf{P}).$$

This allows us to rewrite Eq. (2.6) in the form

$$A(\mathbf{r}, t) = \int a(\mathbf{Q}, \mathbf{P}, \mathbf{r}) F(\mathbf{Q}, \mathbf{P}, t) d\mathbf{Q} d\mathbf{P}, \quad (2.7)$$

where the phase space density  $F$  obeys the celebrated Liouville equation

$$\partial_t F(\mathbf{Q}, \mathbf{P}, t) = -\mathcal{L} F(\mathbf{Q}, \mathbf{P}, t). \quad (2.8)$$

The solutions of Eq. (2.8) are time-independent densities satisfying the relation

$$\{H, F_{eq}\} = 0. \quad (2.9)$$

Every distribution of the form  $F_{eq} = F_{eq}(H(\mathbf{Q}, \mathbf{P}))$  is readily seen to be a solution of Eq. (2.9). We mention in particular the density pertaining to the equilibrium canonical ensemble:

$$F_{eq}(\mathbf{Q}, \mathbf{P}) = \frac{1}{Z} e^{-\beta H(\mathbf{Q}, \mathbf{P})}, \quad (2.10)$$

where  $\beta = 1/(k_B T)$ ,  $k_B$  is Boltzmann's constant,  $T$  is the temperature of the particle system, kept fixed by an external heat bath, and  $Z$  denotes the canonical partition function, which is related to the thermodynamic Helmholtz free energy [2].

In spite of its conceptual relevance, the Liouville equation (2.8) is intractable from a practical point of view, due to the large number of particles. Thus, a more efficient reduced description can be obtained by projecting Eq. (2.8) onto a subspace of the whole phase space. To this end, we introduce the shorthand notation  $\mathbf{z}_i = (\mathbf{q}_i, \mathbf{p}_i)$ . We define the  $s$ -particle marginals  $F_s(\mathbf{z}_1, \dots, \mathbf{z}_s, t)$  as

$$F_s(\mathbf{z}_1, \dots, \mathbf{z}_s, t) = \int F(\mathbf{z}_1, \dots, \mathbf{z}_N, t) \prod_{j=s+1}^N d\mathbf{z}_j, \quad \text{with } j = 1, \dots, N, \quad (2.11)$$

which denotes the probability density of the first  $s$  particles (or of any given group of  $s$  particles) at time  $t$ . To find an equation for the marginal  $F_s$ , we integrate Eq. (2.8) with respect to  $d\mathbf{z}_{s+1}, \dots, d\mathbf{z}_N$ , thus obtaining the so-called BBGKY hierarchy [3], which reads

$$\partial_t F_s = \mathcal{L}_s F_s + \mathcal{C}_{s+1} F_{s+1}, \quad \text{with } s = 1, \dots, N,$$

where

$$\begin{aligned} \mathcal{L}_s F_s &= - \sum_{i=1}^s \mathbf{p}_i \cdot \frac{\partial F_s}{\partial \mathbf{q}_i} + \sum_{i=1}^s \sum_{j=1}^s \frac{\partial \Phi(|\mathbf{q}_i - \mathbf{q}_j|)}{\partial \mathbf{q}_i} \cdot \frac{\partial F_s}{\partial \mathbf{p}_i}, \\ \mathcal{C}_{s+1} F_{s+1} &= (N-s) \sum_{i=1}^s \int d\mathbf{z}_{s+1} \frac{\partial \Phi(|\mathbf{q}_i - \mathbf{q}_{s+1}|)}{\partial \mathbf{q}_i} \cdot \frac{\partial F_{s+1}}{\partial \mathbf{p}_i}. \end{aligned} \quad (2.12)$$

The meaning of Eq. (2.12) is clear: the variation in time of  $F_s$  depends on the interaction of the  $s$  particles among themselves (which is the contribution provided by the operator  $\mathcal{L}_s$ ) and on the interaction of the first  $s$  particles with the rest of the system (represented by the operator  $\mathcal{C}_{s+1}$ ).

Let us also inspect the microscopic dynamical functions more closely. We introduce the one-point *empirical distribution* of the many-particle system, defined as

$$\sum_{i=1}^N \delta(\mathbf{r} - \mathbf{q}_i) \delta(\boldsymbol{\xi} - \mathbf{p}_i), \quad (2.13)$$

where  $\mathbf{r}$  and  $\boldsymbol{\xi}$  are parameters corresponding, respectively, to the position and momentum vectors in the single-particle space. In Sect. 2.2, we will clarify, in particular, in what sense the expression (2.13) is “well represented” by the distribution function entering the Boltzmann equation. Here it suffices to notice that the marginal  $F_1$  is related to the phase space average (2.7) of the one-point empirical distribution (2.13), as follows:

$$\left\langle \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{q}_i) \delta(\boldsymbol{\xi} - \mathbf{p}_i) \right\rangle = N F_1(\mathbf{r}, \boldsymbol{\xi}, t). \quad (2.14)$$

Furthermore, as we will see in Chap. 4, many phase functions of interest are obtained by multiplying the phase space distribution (2.13) by some function of  $\boldsymbol{\xi}$  (see, e.g., Eq. (2.44)) and by integrating over the momentum space [4]. For instance, the local number density  $n(\mathbf{Q}, \mathbf{r})$  reads

$$n(\mathbf{Q}, \mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{q}_i). \quad (2.15)$$

The macroscopic number density  $n(\mathbf{r}, t)$ , which, as discussed in Chap. 3, results from a proper integration of the density  $F_1$  in the single-particle space, can also be derived by taking the ensemble average of the highly discontinuous phase function (2.15) with respect to the phase space density  $F(\mathbf{Q}, \mathbf{P}, t)$ . Analogously, we define the two-point empirical density as

$$\sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \delta(\mathbf{r} - \mathbf{q}_i) \delta(\boldsymbol{\xi} - \mathbf{p}_i) \delta(\mathbf{r}_1 - \mathbf{q}_j) \delta(\boldsymbol{\xi}_1 - \mathbf{p}_j), \quad (2.16)$$

whose phase space average yields  $N(N-1)F_2(\mathbf{r}, \boldsymbol{\xi}, \mathbf{r}_1, \boldsymbol{\xi}_1, t)$ . An integration over the momenta leads to the two-point density function  $n(\mathbf{r}, \mathbf{r}_1, t)$ , which typically differs from the product of the one-point densities  $n(\mathbf{r}, t)n(\mathbf{r}_1, t)$  as long as the distance  $|\mathbf{r} - \mathbf{r}_1|$  is small. The deviation, which stems from the presence of particle interactions, corresponds to the *two-point correlation* [1]. In particular, if we denote by  $V$  the volume of the system, then the two-point function  $n(\mathbf{r}, \mathbf{r}_1)$  for a homogeneous system can be written as

$$n(\mathbf{r}, \mathbf{r}_1) = \left(\frac{N}{V}\right)^2 g^{(2)}(\mathbf{r}, \mathbf{r}_1), \quad (2.17)$$

where the correlation function  $g^{(2)}(\mathbf{r}, \mathbf{r}_1)$  measures the extent to which the structure of a fluid deviates from complete randomness. If the system is also isotropic, then  $g^{(2)}$  depends only on the magnitude of the separation  $s = |\mathbf{r} - \mathbf{r}_1|$ : in this case, the pair correlation function is denoted by  $g(s)$  and is referred to as the *radial distribution function* [5]. By taking the ensemble average of Eq. (2.16), in which the phase space coordinates  $(\mathbf{q}_i, \mathbf{p}_i)$  and  $(\mathbf{q}_j, \mathbf{p}_j)$  are evaluated at two distinct times, say  $t$  and  $t_1$ ,

$$\sum_{i=1}^N \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{q}_i(t)) \delta(\boldsymbol{\xi} - \mathbf{p}_i(t)) \delta(\mathbf{r}_1 - \mathbf{q}_j(t_1)) \delta(\boldsymbol{\xi}_1 - \mathbf{p}_j(t_1)), \quad (2.18)$$

one obtains the two-time joint probability distribution [1]

$$f_2(\mathbf{r}, \boldsymbol{\xi}, t; \mathbf{r}_1, \boldsymbol{\xi}_1, t_1) = N^2 F_2(\mathbf{r}, \boldsymbol{\xi}, t; \mathbf{r}_1, \boldsymbol{\xi}_1, t_1), \quad (2.19)$$

which allows the computation of time correlation functions, whose properties will be explored in Chap. 4.

Before concluding this section, it is instructive to outline some aspects concerning the derivation of the Boltzmann equation for a hard-sphere gas from the hierarchy (2.12). This can be done by taking a proper limit of the time evolution equation for the marginal  $F_1$ . To this end, it is common practice to replace the momentum  $\boldsymbol{\xi}$  with

the velocity  $\mathbf{v}$ . We denote, then, by  $\mathbf{v}$ ,  $\mathbf{v}_1$ ,  $\mathbf{v}'$ , and  $\mathbf{v}'_1$  the precollisional velocities of the two particles in respectively the *direct* and *inverse* encounters (the explicit relations between postcollisional and precollisional velocities will be made clear in Sect. 2.2). Let  $\mathbf{r}$  be the position of the center of the target particle equipped with velocity  $\mathbf{v}$ . In a reference frame centered on the target particle, the latter is at rest and is endowed with twice the actual diameter  $\delta$ . The colliding particle, which is regarded as a point mass equipped with an incoming velocity  $\mathbf{v}_1 - \mathbf{v}$ , hits the so-called *protection* sphere [6] at the point  $\mathbf{r}_1 = \delta \mathbf{n}$ , where  $\mathbf{n}$  is a unit vector, and is contained within a volume  $\delta^2 d\mathbf{n} |(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}| dt$ . The time evolution equation for  $F_1$  attains the form [3, 6]

$$\begin{aligned} \frac{\partial F_1}{\partial t} + \mathbf{v} \cdot \frac{\partial F_1}{\partial \mathbf{r}} &= (N-1) \delta^2 \int \int_{\mathbb{R}^3 S_-} \left[ F_2(\mathbf{r}, \mathbf{v}', \mathbf{r} - \delta \mathbf{n}, \mathbf{v}'_1, t) - F_2(\mathbf{r}, \mathbf{v}, \mathbf{r} + \delta \mathbf{n}, \mathbf{v}_1, t) \right] \\ &\quad \times |(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}| d\mathbf{n} d\mathbf{v}_1, \end{aligned} \quad (2.20)$$

where the integration is over the hemisphere  $S_- = \{\mathbf{n} \in S^2 | (\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n} < 0\}$ . It is worth noticing that the probability densities  $F_2$  in (2.20) are both expressed in terms of the precollisional velocities pertaining respectively to the inverse and the direct encounters. Here, then, is the Boltzmann argument. For a rarefied gas contained in a box with volume  $1 \text{ cm}^3$  at room temperature and atmospheric pressure, we have  $N \simeq 10^{20}$  and  $\delta = 10^{-8} \text{ cm}$ , so that  $(N-1)\delta^2 \simeq N\delta^2 = 1 \text{ m}^2$ ; cf. [3]. The limit  $N \rightarrow \infty$ ,  $\delta \rightarrow 0$ , with  $N\delta^2$  finite, is the so-called Boltzmann–Grad limit; see also Sect. 2.3. In this limit, if each  $F_s$  tends to a limit and this limit is sufficiently smooth, the BBGKY hierarchy (2.12) transforms into the so-called Boltzmann hierarchy [3]. Furthermore, since the volume occupied by the particles corresponds to about  $N\delta^3 \simeq 10^{-4} \text{ cm}^3$ , the collision between two particles is a rather rare event. Thus, the two colliding particles may be thought of as completely uncorrelated *before* the collision, and their joint probability density may be factorized (assumption of *molecular chaos*, or *Stosszahlansatz*) as

$$F_2(\mathbf{r}, \mathbf{v}, \mathbf{r}_1, \mathbf{v}_1, t) = F_1(\mathbf{r}, \mathbf{v}, t) F_1(\mathbf{r}_1, \mathbf{v}_1, t). \quad (2.21)$$

Taking into account the remarks above, one obtains the Boltzmann equation for hard spheres

$$\begin{aligned} \frac{\partial F_1}{\partial t} + \mathbf{v} \cdot \frac{\partial F_1}{\partial \mathbf{r}} &= N\delta^2 \int \int_{\mathbb{R}^3 S_-} \left[ F_1(\mathbf{r}, \mathbf{v}', t) F_1(\mathbf{r}, \mathbf{v}'_1, t) - F_1(\mathbf{r}, \mathbf{v}, t) F_1(\mathbf{r}, \mathbf{v}_1, t) \right] |(\mathbf{v}_1 - \mathbf{v}) \cdot \mathbf{n}| d\mathbf{n} d\mathbf{v}_1. \end{aligned} \quad (2.22)$$

We are not going to dwell further here on the rigorous derivation of the Boltzmann equation, which is beyond the scope of this work. Rather, we wish to outline the heuristic argument that guided Ludwig Boltzmann in the derivation of the celebrated kinetic equation bearing his name.

## 2.2 The Boltzmann Equation

The Boltzmann equation is an evolution equation for the probability density of a given particle, which we denote by  $f(\mathbf{r}, \mathbf{v}, t)$ . This quantity should not be confused in principle with the fraction of molecules located in the cell of size  $d\mathbf{r} \times d\mathbf{v}$  around the point  $\mathbf{r}, \mathbf{v}$ . Although there is no a priori relationship between the two concepts, it can be shown that they are closely related. Let us reformulate this problem in the following manner. As in Sect. 2.1, let us denote by  $\mathbf{z}$  the pair  $(\mathbf{r}, \mathbf{v})$ . Then, given a system of  $N$  identical particles whose physical state is given by the sequence  $\mathbf{z}_1 \dots \mathbf{z}_N$ , we denote by  $F_\Delta(\mathbf{z}_1, \dots, \mathbf{z}_N)$  the fraction of particles localized in a volume  $\Delta$  of the single-particle space, i.e.,

$$F_\Delta(\mathbf{z}_1, \dots, \mathbf{z}_N) = \frac{1}{N} \sum_{i=1}^N \chi_\Delta(\mathbf{z}_i) = \int_\Delta \mu(d\mathbf{z}), \quad (2.23)$$

where  $\chi_\Delta$  is the indicator function and

$$\mu(d\mathbf{z}) = \frac{1}{N} \sum_{i=1}^N \delta(\mathbf{z} - \mathbf{z}_i) d\mathbf{z}$$

is a measure in the single-particle space. In the definition of  $\mu(d\mathbf{z})$  in Eq. (2.2), the reader will also recognize the structure of the empirical distribution, defined in Eq. (2.13). Thus, one may wonder in which sense the random variable  $F_\Delta(\mathbf{z}_1, \dots, \mathbf{z}_N)$  in Eq. (2.23) can be reasonably approximated by

$$\int_\Delta f(\mathbf{z}, t) d\mathbf{z}.$$

It is possible to prove [3] that if  $\mathbf{z}_1, \dots, \mathbf{z}_N$  are independent identically distributed random variables with law  $f(\mathbf{z}, t)$ , then  $\mu(d\mathbf{z})$  is close to  $f(\mathbf{z}, t) d\mathbf{z}$ , in a sense specified by the law of large numbers, when  $N$  diverges. That is, the Boltzmann equation refers to the limiting situation such that the many-particle system specified by the sequence  $\mathbf{z}_1, \dots, \mathbf{z}_N$  can be actually considered a large number of copies of independent single-particle systems for which  $\mu(d\mathbf{z})$  and  $f(\mathbf{z}) d\mathbf{z}$  can be regarded as the same object. Moreover, it is common to rescale  $f(\mathbf{z}, t)$  by setting

$$f(\mathbf{r}, \mathbf{v}, t) = N F_1(\mathbf{r}, \mathbf{v}, t), \quad (2.24)$$

cf. Eq. (2.14). The quantity  $f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}$  is to be regarded as the *average* number of particles contained in the element  $d\mathbf{r} d\mathbf{v}$  at a given time  $t$ , when the fluctuations which occur in a short time interval  $dt$  are neglected [7]. The definition of the function  $f$  relies, hence, on probability concepts, and hereinafter, we will tacitly assume that the

macroscopic variables computed from the knowledge of the distribution function  $f$  at a certain time  $t$  result from an average over the time interval  $dt$  around  $t$ . We will return in more detail to this issue in Sect. 3.1. It is worth mentioning that the role of fluctuations in the single-particle space was the subject of a research investigation [8–10] that led to the construction of a fluctuating Boltzmann equation that recovers the standard Boltzmann equation on average and from which the macroscopic equations of fluctuating hydrodynamics [11] can be derived.

Let us now outline some basic aspects concerning the geometry of an elastic collision between two particles endowed with equal mass  $m$ .

We consider the scattering of a particle, labeled 2, equipped with velocity  $\mathbf{v}_1$ , induced by the *target* particle labeled 1, with velocity  $\mathbf{v}$ . The pre- and postcollisional velocities are related by momentum and kinetic energy conservation:

$$\begin{aligned}\mathbf{v} + \mathbf{v}_1 &= \mathbf{v}' + \mathbf{v}'_1, \\ \mathbf{v}^2 + \mathbf{v}_1^2 &= \mathbf{v}'^2 + \mathbf{v}'_1{}^2.\end{aligned}\tag{2.25}$$

Introducing the center-of-mass variables

$$\begin{aligned}\mathbf{G} &= \frac{1}{2}(\mathbf{v} + \mathbf{v}_1), \\ \mathbf{g} &= \mathbf{v}_1 - \mathbf{v},\end{aligned}$$

and the corresponding variables  $\mathbf{G}'$  and  $\mathbf{g}'$  for the postcollisional velocities (in the direct encounter), the conservation equations (2.25) yield  $g = g'$ , where  $g \equiv |\mathbf{g}|$ . Hence, the relative velocity is changed by the collision only in direction and not in magnitude.

We consider, then, a reference frame in which the target particle is at rest. In this frame, the geometry of the scattering is determined by the collision (unit) vector  $\mathbf{n}$ , which forms an angle  $\theta$ , called the collision angle, with the direction of  $\mathbf{g}$  and halves the angle between  $\mathbf{g}$  and  $\mathbf{g}'$ ; cf. Fig. 2.1. Therefore, in the direct encounter, the precollisional and postcollisional velocities, respectively  $\mathbf{g}$  and  $\mathbf{g}'$ , are related by

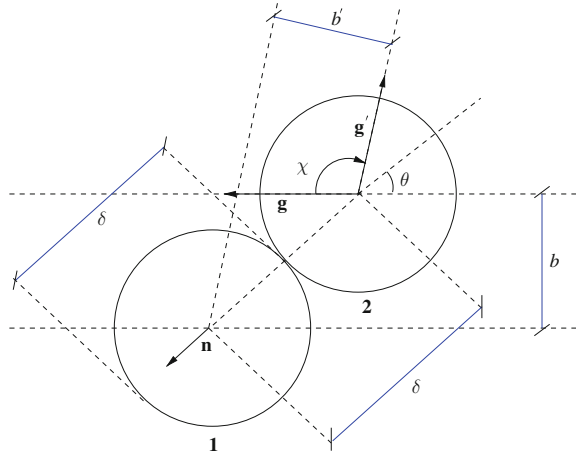
$$\mathbf{g} - \mathbf{g}' = 2(\mathbf{g} \cdot \mathbf{n})\mathbf{n}.\tag{2.26}$$

Using (2.26), it is possible to derive the following relations between pre- and postcollisional velocities:

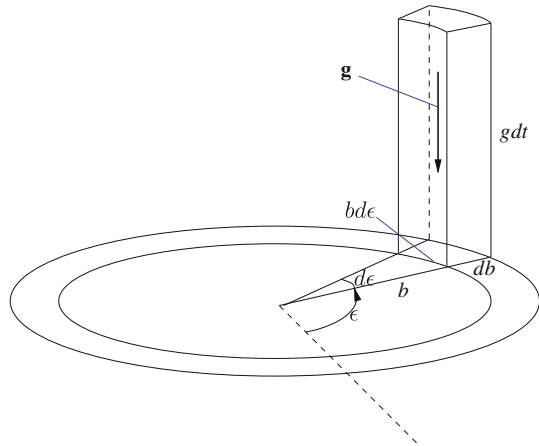
$$\begin{aligned}\mathbf{v}' - \mathbf{v} &= (\mathbf{g} \cdot \mathbf{n})\mathbf{n}, \\ \mathbf{v}'_1 - \mathbf{v}_1 &= -(\mathbf{g} \cdot \mathbf{n})\mathbf{n}.\end{aligned}\tag{2.27}$$

the relations (2.27) show that the dynamical effect of the encounter is known when the direction of the unit vector  $\mathbf{n}$  is also determined. Yet the latter vector cannot be computed by relying only on the balance equation (2.25), because there are two

**Fig. 2.1** Scattering kinematics for hard *spheres*, with precollisional relative velocity  $\mathbf{g}$ , postcollisional velocity  $\mathbf{g}'$ , impact parameter  $b$ , collision angle  $\theta$ , and collision vector  $\mathbf{n}$ .



**Fig. 2.2** Collision cylinder for particles with relative velocity  $\mathbf{g}$  that collide with the target particle during a time interval  $dt$ .



geometric variables to be specified. The first is the azimuthal angle  $\epsilon$ , describing the orientation of the plane containing  $\mathbf{g}$  and  $\mathbf{g}'$  (which lie in the same plane, as specified below) with a reference plane; cf. Fig. 2.2.

The second geometric variable of the encounter is the impact parameter  $b$ , which corresponds to the perpendicular distance between the center of the target particle 1 and the original line of motion of the scattered particle 2, identified by the relative velocity  $\mathbf{g}$ , as shown in Fig. 2.1. Moreover, the angle of deflection  $\chi = \pi - 2\theta$  is, in general, a function of  $g$  and of  $b$ , with a specific functional relation  $\chi(g, b)$  that depends on the particle interaction potential (see below). Analogously, one may also introduce the postcollisional impact parameter  $b'$ , defined with respect to the velocity  $\mathbf{g}'$ , as illustrated in Fig. 2.1. The conservation of the angular momentum entails that the collision takes place in a plane, called the *collision plane*, and yields  $b = b'$ .

Let us now focus on the statistics of the encounters. To this end, we use, for simplicity, the abbreviations  $f \equiv f(\mathbf{r}, \mathbf{v}, t)$ ,  $f_1 \equiv f(\mathbf{r}, \mathbf{v}_1, t)$ ,  $f' \equiv f(\mathbf{r}, \mathbf{v}', t)$ , and  $f'_1 \equiv f(\mathbf{r}, \mathbf{v}'_1, t)$ . The collision between the target particle 1 and an arbitrary particle 2 occurs if the latter is located within the cylinder with volume  $dV = (gdt)(bdbd\varepsilon)$  shown in Fig. 2.2. The (average) number of the particles 2 equipped with a velocity in the range  $[\mathbf{v}_1, \mathbf{v}_1 + d\mathbf{v}_1]$  and located in any such cylinders is given by  $f_1 d\mathbf{v}_1 dV$ . We can imagine such a cylinder to be associated with any of the particles 1, so that the total number of encounters, under the assumption of molecular chaos considered by Boltzmann, is given by

$$f d\mathbf{v} d\mathbf{r} f_1 d\mathbf{v}_1 (gdt)(bdbd\varepsilon). \quad (2.28)$$

The surface element  $bdbd\varepsilon$  in Eq. (2.28) can be written in terms of the element  $d\mathbf{n} = \sin \theta d\theta d\varepsilon$ , using the relation

$$bdbd\varepsilon = \sigma(g, b) d\mathbf{n}. \quad (2.29)$$

The quantity  $\sigma(g, b)$  in Eq. (2.29) is called the differential scattering cross section and is defined by the relation

$$\sigma(g, b) = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right|. \quad (2.30)$$

It contains all the detailed information on the particle interactions [3, 6, 7]. In particular, by assuming, as above, that the interaction potential  $\Phi(s)$  depends only on the magnitude of the relative distance  $s = |\mathbf{r} - \mathbf{r}_1|$  between the particles, the specific functional relation among  $\theta$ ,  $g$ , and  $b$  can be obtained from the general relation

$$\theta(g, b) = \int_0^{z^*} \frac{dz}{\sqrt{1 - z^2 - \frac{4\Phi(b/z)}{mg^2}}}, \quad \text{with } 1 - z^{*2} - \frac{4\Phi(b/z^*)}{mg^2} = 0. \quad (2.31)$$

Here  $z = b/s$  is a dimensionless inverse distance, and  $z^*$  denotes its value at the minimum particle distance  $s_{\min}$ . Equation (2.31) provides the fundamental relationship  $\theta(b, g)$ . Inverting this relation, one obtains  $b(\theta, g)$ , which thus yields  $\sigma(g, \theta)$  as a function of  $g$  and  $\theta$ . In particular, for hard spheres of diameter  $\delta$ , as shown in Fig. 2.1, the relation  $b = \delta \sin \theta$  holds. This yields

$$\sigma_{HS}(g, \theta) = \delta^2 \cos \theta, \quad (2.32)$$

which hence shows that for a hard-sphere gas, the scattering cross section depends only on  $\theta$ . On the other hand, for power law potentials of the form  $\Phi(s) = \Phi_0 s^{(1-n)}$ ,

with  $\Phi_0$  and  $n$  constants, we have

$$\sigma_n(g, \theta) = \beta(\theta) g^{-\frac{4}{n-1}}, \quad (2.33)$$

where  $\beta(\theta)$  is a function of  $\theta$  alone [6]. The case  $n = 5$  occupies a distinct place in the Boltzmann equation theory, since it allows a considerable simplification: in this case, the product  $g\sigma(g, \theta)$ , which enters the expression of the collision operator (to be made explicit below, cf. Eq. (2.41)) depends only on  $\theta$ . This result was discovered by Maxwell, whence the fictitious molecules interacting via such a purely repulsive potential are called Maxwell molecules [6]. We will return to Maxwell molecules in Chap. 5, to discuss the derivation of hydrodynamics from kinetic models of the Boltzmann equation.

In the inverse encounters, characterized by pre- and postcollisional velocities given, respectively, by  $\mathbf{v}', \mathbf{v}'_1$  and  $\mathbf{v}, \mathbf{v}_1$ , the differential scattering cross section is a function of  $g'$  and  $b'$ . Using the relations  $g = g'$  and  $b = b'$ , one immediately obtains

$$\sigma(g', b') = \sigma(g, b), \quad (2.34)$$

which reflects the time reversibility of the collisional event. In particular, we recall that the scattering cross section  $\sigma$  is related to the conditional probability density  $W(\mathbf{v}', \mathbf{v}'_1 | \mathbf{v}, \mathbf{v}_1)$  of a collision that, in the direct encounter, carries the two particles from the velocities  $\mathbf{v}$  and  $\mathbf{v}_1$  into the velocities  $\mathbf{v}'$  and  $\mathbf{v}'_1$  [6, 12]. The explicit relation between  $W$  and  $\sigma$  reads

$$W(\mathbf{v}', \mathbf{v}'_1 | \mathbf{v}, \mathbf{v}_1) = 2m^4 \frac{\sigma(g, \theta)}{\cos \theta} \delta(\mathbf{v} + \mathbf{v}_1 - \mathbf{v}' - \mathbf{v}'_1) \delta(\mathbf{v}^2 + \mathbf{v}_1^2 - \mathbf{v}'^2 - \mathbf{v}'_1^2), \quad (2.35)$$

where the two delta functions ensure the conservation of the momentum and of the kinetic energy. Moreover, from (2.34) and (2.35), it follows that

$$W(\mathbf{v}', \mathbf{v}'_1 | \mathbf{v}, \mathbf{v}_1) = W(\mathbf{v}, \mathbf{v}_1 | \mathbf{v}', \mathbf{v}'_1), \quad (2.36)$$

which is another expression of the time reversibility of the collisional event. The conditional probability density is also symmetric under the exchange of particles

$$W(\mathbf{v}, \mathbf{v}_1 | \mathbf{v}', \mathbf{v}'_1) = W(\mathbf{v}_1, \mathbf{v} | \mathbf{v}'_1, \mathbf{v}'). \quad (2.37)$$

Let us now consider the set of particles located within  $d\mathbf{r}$  and with velocities in the range  $[\mathbf{v}, \mathbf{v} + d\mathbf{v}]$ , and let us also denote by  $L$  and  $G$  the negative and positive contributions to the variation of  $f$  due to the collisions. The loss term  $L$  can be computed by considering the direct encounter in which the precollisional velocities  $\mathbf{v}, \mathbf{v}_1$  transform, according to Eq. (2.27), into the postcollisional ones. Therefore, using (2.28), one can write

$$L = f f_1 g \sigma(g, b) d\mathbf{n} d\mathbf{v} d\mathbf{v}_1 d\mathbf{r} dt. \quad (2.38)$$

The gain term  $G$  can be found in a similar manner by considering inverse encounters. The relation between pre- and postcollisional velocities in the inverse encounter follows directly from Eq. (2.27) on interchanging  $\mathbf{v}$ ,  $\mathbf{v}_1$  and  $\mathbf{v}'$ ,  $\mathbf{v}'_1$ , and by replacing  $\mathbf{n}$  by  $(-\mathbf{n})$  and  $\mathbf{g}$  by  $\mathbf{g}'$  [7]. Thus, one obtains

$$G = f' f'_1 g' \sigma(g', b') d\mathbf{n} d\mathbf{v}' d\mathbf{v}'_1 d\mathbf{r} dt. \quad (2.39)$$

Since the Jacobian of the transformation from precollisional to postcollisional velocities is unitary, i.e.,  $d\mathbf{v} d\mathbf{v}_1 = d\mathbf{v}' d\mathbf{v}'_1$ , and because of Eq. (2.34), we can use  $g \sigma(g, b) d\mathbf{v} d\mathbf{v}_1$  also in (2.39). Dividing both terms  $L$  and  $G$  by  $d\mathbf{v} d\mathbf{r} dt$  and performing the integration over the variables  $\mathbf{v}_1$  and  $\mathbf{n}$ , we obtain the Boltzmann equation in absence of external forces:

$$\partial_t f(\mathbf{r}, \mathbf{v}, t) + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = Q(f, f), \quad (2.40)$$

where

$$Q(f, f) = \int \int \left( f' f'_1 - f f_1 \right) g \sigma(g, \theta) d\mathbf{n} d\mathbf{v}_1 \quad (2.41)$$

denotes a nonlinear integral collision operator. In particular, using the expression (2.32) of the scattering cross section for hard spheres, one readily recovers Eq. (2.22). We recall that the integration over  $\mathbf{n}$  corresponds to a double integration over  $\varepsilon = [0, 2\pi]$  and  $\theta = [0, \pi/2]$ ; cf. Fig. 2.1. Alternatively, the collision operator can be expressed in terms of the conditional probability densities introduced in Eq. (2.35), and using (2.36), it attains the form

$$Q(f, f) = \int \int \int \left( f' f'_1 - f f_1 \right) W(\mathbf{v}, \mathbf{v}_1 | \mathbf{v}', \mathbf{v}'_1) d\mathbf{v}_1 d\mathbf{v}' d\mathbf{v}'_1, \quad (2.42)$$

which is sometimes referred to as the *quasichemical* representation.

A basic property of the operator (2.41), which will be employed in the sequel of this work, concerns the conservation of mass, momentum, and kinetic energy of the particles during the collisions. Defining the vector of the so-called *elementary collision invariants* as

$$\psi(\mathbf{v}) = [\Psi_1, \psi_2, \Psi_3], \quad (2.43)$$

with

$$\Psi_1 = m, \quad \psi_2 = m\mathbf{v}, \quad \Psi_3 = \frac{m}{2} v^2, \quad (2.44)$$

and  $v \equiv |\mathbf{v}|$ , one obtains the important relation

$$\int Q(f, f) \psi(\mathbf{v}) d\mathbf{v} = \mathbf{0}, \quad (2.45)$$

which expresses the conservation of the mean values of mass, momentum, and kinetic energy of the particles during the collisions; cf. Sect. 3.1. In general, any function  $\Phi(\mathbf{r}, \mathbf{v}, t)$  satisfying the relation

$$\phi'_1 + \phi' = \phi_1 + \phi \quad (2.46)$$

is a collision invariant and can be written as a linear combination of the elements of  $\psi(\mathbf{v})$ .

### 2.2.1 *H-Theorem and the Maxwellian Distribution*

Let us consider a uniform gas in the absence of external forces. In this case, the Boltzmann equation (2.40) reads

$$\partial_t f(\mathbf{r}, \mathbf{v}, t) = \iint (f' f'_1 - f f_1) g \sigma(g, \theta) d\mathbf{n} d\mathbf{v}_1. \quad (2.47)$$

Furthermore, let  $H$  be the complete integral (i.e., the integral over all values of velocities) defined by the equation

$$H(t) = \int f \log f d\mathbf{v}. \quad (2.48)$$

By computing the time derivative of the  $H$ -function defined in Eq. (2.48) through Eq. (2.47), one obtains

$$\partial_t H(t) = \frac{1}{4} \iiint g \sigma (f' f'_1 - f f_1) \ln \left( \frac{f f_1}{f' f'_1} \right) d\mathbf{v} d\mathbf{v}_1 d\mathbf{n}. \quad (2.49)$$

The structure of Eq. (2.49) leads to the following inequality, called the *H-theorem*:

$$\partial_t H(t) \leq 0. \quad (2.50)$$

Equation (2.50) shows that the function  $H(t)$  decreases monotonically over time. Consequently, the particle system keeps no track of its initial distribution, and is driven toward a final state described by the distribution  $f^{\text{GM}}$ . The latter satisfies the relation

$$f^{\text{GM}}(\mathbf{v}) f^{\text{GM}}(\mathbf{v}_1) = f^{\text{GM}}(\mathbf{v}') f^{\text{GM}}(\mathbf{v}'_1). \quad (2.51)$$

Taking the logarithm of both sides of (2.51), we obtain a relation of the form (2.46):  $\ln f^{\text{GM}}$  is a collision invariant and hence can be written as a sum of the elementary collision invariants (2.44):

$$\ln f^{\text{GM}}(\mathbf{v}) = \alpha_1 + \alpha_2 \cdot m\mathbf{v} + \alpha_3 \frac{m}{2} v^2.$$

The coefficients  $\alpha_1, \alpha_2, \alpha_3$  are determined by ensuring that the distribution  $f^{\text{GM}}$  yields the proper values for the mass density, momentum density, and internal energy density, denoted respectively by  $\rho_0, \mathbf{u}_0, T_0$ , with  $\rho_0 = mn_0$ :

$$\begin{aligned} \int f^{\text{GM}} d\mathbf{v} &= \rho_0, \\ \int f^{\text{GM}} \mathbf{v} d\mathbf{v} &= \rho_0 \mathbf{u}_0, \\ \frac{m}{2} \int f^{\text{GM}} (\mathbf{v} - \mathbf{u})^2 d\mathbf{v} &= \frac{3}{2} n_0 k_B T_0. \end{aligned} \quad (2.52)$$

Therefore, the general equilibrium distribution attains the form

$$f^{\text{GM}}(\mathbf{v}) = n_0 \left( \frac{m}{2\pi k_B T_0} \right)^{\frac{3}{2}} e^{-\frac{m(\mathbf{v} - \mathbf{u}_0)^2}{2k_B T_0}}. \quad (2.53)$$

If the macroscopic fields  $n, \mathbf{u}, T$  depend on  $\mathbf{r}$  and  $t$ , the corresponding equilibrium distribution is then referred to as the *local Maxwellian*, and it reads

$$f^{\text{LM}}(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r}, t) \left( \frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} e^{-\frac{m(\mathbf{v} - \mathbf{u}(\mathbf{r}, t))^2}{2k_B T(\mathbf{r}, t)}}. \quad (2.54)$$

The expression (2.54) represents an important reference distribution for describing a gas's behavior in close-to-equilibrium regimes.

## 2.3 Hydrodynamic Limit and Other Scalings

A point of remarkable interest in kinetic theory concerns the study of the scaling properties of the Boltzmann equation. In particular, one may investigate the structure of the solutions of the Boltzmann equation in the so-called *hydrodynamic limit*, which is obtained by taking the limits  $N \rightarrow \infty, V \rightarrow \infty$ , with  $N/V$  finite, where  $N$  is the total number of particles in a box  $\Lambda_\varepsilon$  with volume  $V$ . Following the approach given in [3], let us introduce a small parameter  $\varepsilon$ , and let the side of the box  $\Lambda_\varepsilon$  be proportional to  $\varepsilon^{-1}$ . Let  $f^\varepsilon(\mathbf{r}, \mathbf{v}, t)$ , with  $\mathbf{r} \in \Lambda_\varepsilon$ , be the number density of the particles in the box. Then we assume that the total number of particles is proportional to the volume of the box

$$\int_{\Lambda_\varepsilon \times \mathbb{R}^3} f^\varepsilon(\mathbf{r}, \mathbf{v}) d\mathbf{r} d\mathbf{v} = \varepsilon^{-3}, \quad (2.55)$$

and introduce the following scaling:

$$\hat{\mathbf{r}} = \varepsilon \mathbf{r}, \quad \tau = \varepsilon t, \quad (2.56)$$

with  $\mathbf{r} \in \Lambda = [0, 1]$ , and

$$\hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau) = f^\varepsilon(\mathbf{r}, \mathbf{v}, t). \quad (2.57)$$

It is readily seen that the rescaled distribution  $\hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau)$  can suitably describe the particle system on the scale of the box and is normalized to unity:

$$\int_{\Lambda \times \mathbb{R}^3} \hat{f}(\hat{\mathbf{r}}, \mathbf{v}) d\hat{\mathbf{r}} d\mathbf{v} = 1. \quad (2.58)$$

As discussed in [3], while the description in terms of the distribution  $f^\varepsilon$  is called *microscopic*, the description given by the rescaled distribution  $\hat{f}$  can be defined as *macroscopic*, since it provides a statistical description of the particle system on large length and time scales. From (2.56) and (2.57), the Boltzmann equation, in the absence of external forces, attains the structure

$$\partial_\tau \hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau) + \mathbf{v} \cdot \nabla_{\hat{\mathbf{r}}} \hat{f} = \frac{1}{\varepsilon} Q(\hat{f}, \hat{f}), \quad (2.59)$$

which will be the starting point of the methods of reduced description treated in Chap. 3. We expend a few words now on another scaling, in order to clarify the nature of the Boltzmann–Grad limit, introduced earlier. As mentioned in Sect. 2.1, the Boltzmann–Grad limit corresponds to taking the limits  $N \rightarrow \infty$ ,  $\delta \rightarrow 0$ , with  $N\delta^2$  finite. If we now take  $\varepsilon = \delta$ , we require the particle number to be of order  $\varepsilon^{-2}$ , i.e., it goes with the power 2/3 of the volume:

$$\int_{\Lambda_\varepsilon \times \mathbb{R}^3} f^\varepsilon(\mathbf{r}, \mathbf{v}) d\mathbf{r} d\mathbf{v} = \varepsilon^{-2}. \quad (2.60)$$

Next, if we employ the scaling (2.56) and wish to keep the normalization of  $\hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau)$  to unity as in Eq. (2.58), we resort to a different scaling, given by

$$\hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau) = \varepsilon^{-1} f^\varepsilon(\mathbf{r}, \mathbf{v}, t). \quad (2.61)$$

Hence, the Boltzmann equation for the distribution  $\hat{f}$  reads

$$\partial_\tau \hat{f}(\hat{\mathbf{r}}, \mathbf{v}, \tau) + \mathbf{v} \cdot \nabla_{\hat{\mathbf{r}}} \hat{f} = Q(\hat{f}, \hat{f}). \quad (2.62)$$

Equation (2.62) is invariant under the scalings (2.56) and (2.61). It is also clear why the Boltzmann–Grad limit corresponds to a *low-density* limit: in this limit, in fact, the ratio of the particle number to the volume tends to zero [3]. The introduction

of the parameter  $\varepsilon$  in the scaling (2.56) reflects the existence of different length and time scales in a gas. In particular, the structure of the hydrodynamic equations derived from the Boltzmann equation strongly depends on the magnitude of  $\varepsilon$ , which determines the appropriate gas dynamic regime.

As will also be discussed in Chap. 3, the presence of a definite time scale separation in an inhomogeneous gas allows us to construct the following representation of the relaxation to equilibrium: starting from an arbitrary nonequilibrium initial state, the sequence of collisions characterized by the time scale  $\tau_{mf}$  (the mean time between collisions) triggers the evolution of the system toward the local equilibrium regime, which is reached in a “mesoscopic” time interval  $\Delta t$ . From then onward, one may assign locally a value to the macroscopic fields  $\rho, \mathbf{u}, T$ , which also then evolve according to a characteristic time scale  $\tau_{\text{macro}}$ . Then in the final stage of the relaxation process, the slow dynamics of the macroscopic variables drives the particle system toward the final, homogeneous, equilibrium state (2.53).

## 2.4 Linearized Collision Integrals and Kinetic Models

One of the major shortcomings of the Boltzmann equation (2.40) concerns the nonlinear nature of the integral collision operator, which is traced back to the assumption of molecular chaos. The Maxwellian distributions introduced in Sect. 2.2.1 represent a first step in the description of a particle system: they describe equilibrium states characterized by the absence of dissipation. In going beyond equilibrium, one has to rely on approximation methods such as perturbation techniques: one typically expands the distribution function  $f$  in powers of the aforementioned parameter  $\varepsilon$ , which in certain favorable situations can be considered to be small. We focus here on the properties of the collision operator  $Q(f, f)$  under such perturbation theory. Near global equilibrium, one can split the distribution function into the sum of two contributions:

$$f(\mathbf{r}, \mathbf{v}, t) = f^{\text{GM}}(\mathbf{v}) + \Delta f(\mathbf{r}, \mathbf{v}, t), \quad (2.63)$$

where  $\Delta f(\mathbf{r}, \mathbf{v}, t) = f^{\text{GM}}(\mathbf{v})h(\mathbf{r}, \mathbf{v}, t)$  represents a “small” deviation from the equilibrium distribution. By linearizing the Boltzmann collision operator around equilibrium, one obtains the *linearized* collision operator  $L$ ,

$$Lh = 2 \left( f^{\text{GM}} \right)^{-1} Q(f^{\text{GM}}, \Delta f) = \int f^{\text{GM}}(\mathbf{v}_1) \left( h'_1 + h' - h_1 - h \right) g \sigma(g, \theta) d\mathbf{n} d\mathbf{v}_1, \quad (2.64)$$

where  $\sigma(g, \theta)$  contains, as seen above, the details of the particle interactions. Then, by introducing the Hilbert space  $\mathcal{H}$  endowed with scalar product  $\langle g|h \rangle$  and norm  $\|h\|$  defined by

$$\langle g|h \rangle = \frac{1}{n_0} \int f^{\text{GM}}(\mathbf{v}) g(\mathbf{v}) h(\mathbf{v}) d\mathbf{v}, \quad \|h\|^2 = \langle h|h \rangle, \quad (2.65)$$

one finds that the operator  $L$  in Eq. (2.64) is self-adjoint, i.e.,

$$\langle g|Lh \rangle = \langle Lg|h \rangle.$$

Moreover, by setting  $g = h$  in (2.64), one also obtains

$$\langle h|Lh \rangle = -\frac{1}{4} \int |h'_1 + h' - h_1 - h|^2 g \sigma(g, \theta) d\mathbf{n} d\mathbf{v}_1 d\mathbf{v} \leq 0, \quad (2.66)$$

where equality holds if and only if  $h$  is a collision invariant. A simple problem for the linearized operator  $L$  concerns the asymptotic behavior of a homogeneous gas, prepared in an initial state slightly deviating from equilibrium and described by a distribution of the form (2.63). In this case, one studies the linearized Boltzmann equation

$$\partial_t h = Lh. \quad (2.67)$$

If  $h$  is such that  $\|h\|$  and  $\langle h|Lh \rangle$  exist, then from (2.66), one obtains

$$\partial_t \left[ \frac{1}{2} \|h\|^2 \right] = \langle h|Lh \rangle \leq 0,$$

which entails that  $\|h(t_2)\| \leq \|h(t_1)\|$  for  $t_2 > t_1$ , where equality holds if  $h$  is a collision invariant. Moreover, if  $f$  is chosen to have the same density, bulk velocity, and temperature of  $f^{\text{GM}}$  as in Eqs. (2.52), then

$$\langle \psi|h \rangle = 0, \quad (2.68)$$

and the only collision invariant that satisfies these relations is  $h = 0$ . Therefore,  $\|h(t)\|$  decreases until it vanishes for  $t \rightarrow \infty$ . We also mention here that another remarkable problem concerns the study of the spectrum of  $L$  [6], i.e., the set of eigenvalues  $\lambda$  of  $L$  for which  $(L - \lambda I)^{-1}$  is not a bounded operator in  $\mathcal{H}$  or is not uniquely determined. This aspect will be elaborated in Chap. 5.

A complementary strategy to simplify the complicated structure of the Boltzmann equation consists in providing simpler expressions for the collision operator, which, in spite of neglecting many details about the particle interactions, allow one to retain the basic properties of the original collision operator. This is the philosophy behind the wealth of kinetic models proposed in the literature. The simplest example is represented by the BGK model [13–15], which reads

$$\partial_t f + \mathbf{v} \cdot \nabla_r f = -\nu(f - f^{\text{LM}}), \quad (2.69)$$

where  $\nu$  denotes the mean collision frequency, independent of the microscopic velocity  $\mathbf{v}$ . The BGK collision operator in Eq. (2.69) is a nonlinear operator: the nonlinearity occurs because the local Maxwellian  $f^{\text{LM}}$  is parameterized by the values of the fields  $\rho$ ,  $\mathbf{u}$ ,  $T$ , which are obtained by integrating the distribution function itself, as also shown in Eqs. (2.52). In the applications, the linearized version of the BGK operator is mostly used. Considering small deviations from global equilibrium characterized by the values  $[\rho_0, \mathbf{u}_0 = 0, T_0]$ , the linearized BGK collision operator attains the form

$$L_{\text{BGK}} = -\nu \left[ h - \langle \tilde{\psi} | h \rangle \tilde{\psi}(\mathbf{c}) \right], \quad (2.70)$$

where  $\mathbf{c} = \mathbf{v}/v_T$  is the dimensionless peculiar velocity and  $v_T = \sqrt{2k_B T_0/m}$  is the equilibrium thermal velocity. The functions  $\tilde{\psi}(\mathbf{c}) = [\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3]$  read

$$\tilde{\psi}(\mathbf{c}) = \left[ 1, \sqrt{2}\mathbf{c}, \sqrt{\frac{2}{3}} \left( c^2 - \frac{3}{2} \right) \right], \quad (2.71)$$

and they are mutually orthonormal with respect to the scalar product defined in Eq. (2.65). Equation (2.70) can also be formally written in the form

$$L_{\text{BGK}} = -\nu [1 - P_0] h, \quad (2.72)$$

where  $P_0$  denotes the projection operator onto the subspace of  $\mathcal{H}$  spanned by the functions  $\tilde{\psi}$ .

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