

# Large scale dynamics of dilute gases

– Very preliminary version –

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# Chapter 1

## Introduction

### 1.1 Introduction

### 1.2 Equilibrium statistical mechanics

A gas or a liquid at equilibrium can be described in terms of a few macroscopic variables as the pressure  $P$ , the volume  $V$  and the temperature  $T$ . These parameters obey well established physical laws, for example  $PV = nRT$  for an ideal gas, and the different phases of a system are determined by these parameters (see Figure 1.1).

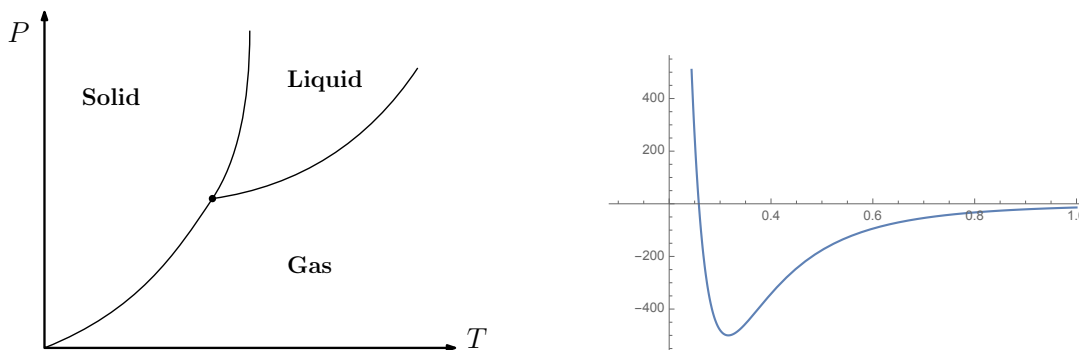


Figure 1.1: The left figure represents a phase diagram. The Lennard-Jones potential (1.2) is depicted on the right. The potential is tuned such that the particles repel at short distances and attract each other otherwise.

A gas is made of a huge number of interacting atoms  $N \approx 10^{23}$  and the goal of statistical mechanics is to derive the macroscopic laws of physics starting from the microscopic interactions between the atoms. To model a gas, the positions and the velocities of the atoms can be encoded by the variables  $\{(x_i, v_i)\}_{i \leq N}$  which are randomly distributed according to the Gibbs theory described next. The kinetic energy of a gas is a function of the velocities  $V_N = \{v_i\}_{i \leq N}$

$$H_{kinetic}(V_N) = \frac{m}{2} \sum_{i=1}^N v_i^2, \quad (1.1)$$

where  $m$  stands for the mass of an atom. The particle interactions depend on an interaction potential  $\Phi$  often represented by a Lennard-Jones potential of the form (see Figure 1.1)

$$r \geq 0, \quad \Phi(r) = E_0 \left( \frac{1}{r^{12}} - \frac{1}{r^6} \right), \quad (1.2)$$

for some constant  $E_0 > 0$ . An additional parameter  $\varepsilon > 0$  is introduced to fix the typical distance between the atoms. As a consequence, the potential  $\Phi$  is rescaled in order to define the interaction energy which depends only on the positions  $X_N = \{x_i\}_{i \leq N}$

$$H_{interaction}(X_N) = \sum_{\substack{i,j \\ i \neq j}} \Phi \left( \frac{x_i - x_j}{\varepsilon} \right). \quad (1.3)$$

The energy between two atoms is minimal when their distance is of order  $\varepsilon$  and their interaction becomes negligible if their distance is much larger than  $\varepsilon$ . To fix ideas, we assume that the gas is contained in a macroscopic vessel modelled by the unit domain  $\mathbb{T}^3 = [0, 1]^3$  so that each  $x_i$  takes values in  $\mathbb{T}^3$ . In order to disregard the boundary effects, the vessel is assumed to be periodic.

Gibbs theory is the cornerstone of statistical mechanics as it relates the macroscopic parameters to statistical averages of some microscopic observables. At equilibrium the atom coordinates  $Z_N = \{X_N, V_N\}$  are distributed according to the *Gibbs measure* with density

$$\mathcal{G}_{N,\beta}(Z_N) = \frac{1}{\mathcal{Z}_{N,\beta}} \exp \left( -\beta \left( H_{kinetic}(V_N) + H_{interaction}(X_N) \right) \right), \quad (1.4)$$

with respect to the Lebesgue measure  $dx_1 \dots dx_N dv_1 \dots dv_N$  in  $(\mathbb{T}^3 \times \mathbb{R}^3)^N$ . At equilibrium, the thermodynamic parameters can be recovered by averaging microscopic variables with respect to the Gibbs measure. Since the Gibbs measure is translation invariant, the density of the gas is simply given by

$$\rho = N\varepsilon^d. \quad (1.5)$$

The temperature is defined by

$$T = \frac{m}{3} \mathbb{E}_{\mathcal{G}_{N,\beta}}(v_i^2) = \frac{1}{\beta}. \quad (1.6)$$

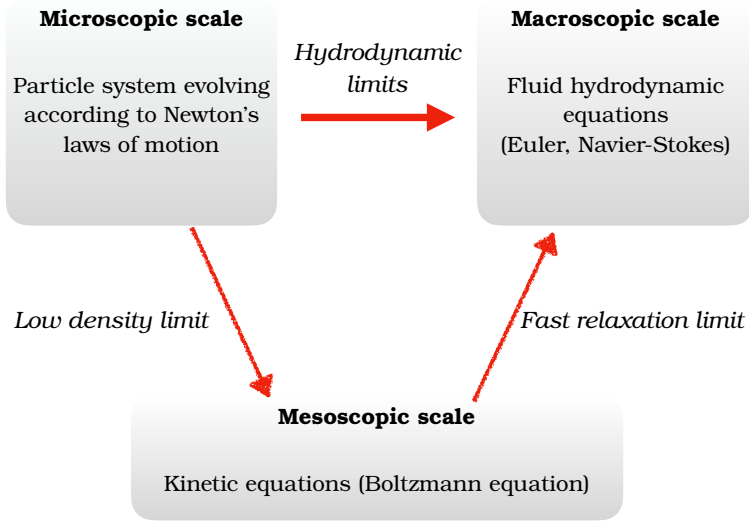
Further macroscopic parameters can be recovered by computing atom correlations under the Gibbs measure. The Gibbs theory relates the microscopic and macroscopic scales in the thermodynamic limit, i.e. when the particle number  $N$  tends to infinity and  $\varepsilon$  tends to 0 in such a way that the density is kept fixed

$$\rho = \lim_{\substack{N \rightarrow \infty, \\ \varepsilon \rightarrow 0}} N\varepsilon^d. \quad (1.7)$$

From a probabilist view point, this limit should be interpreted as a law of large numbers which ensures that averages of a random sequence are close to a mean behavior. As the particle number in a gas is typically of order  $10^{23}$ , the limiting regime provides an accurate description of the gas. Physical laws at equilibrium can be deduced from the Gibbs theory and, in particular, the phase diagram can be predicted from the microscopic description (even so, this has not been achieved yet by a fully rigorous mathematical theory).

### 1.3 Hydrodynamic limits

In every day life, most of the physical systems are out-of-equilibrium and one would like to derive the laws of non-equilibrium physics from the microscopic particle systems. In particular, one of the great challenge would be to recover the hydrodynamic equations from Newton's laws of motion governing the (classical) atom dynamics. In this section, we will review the different levels of description of a gas and their relations by scaling limits.



At a macroscopic scale, a gas can be seen as a continuous substance described by a few parameters varying in time and space: the local density  $\rho(\tau, r)$ , the local velocity  $u(\tau, r)$  and the local temperature  $T(\tau, r)$  (which is related to the local energy). Depending on the physical regimes, the evolution of the field  $(\rho, v, T)$  follows different hydrodynamic equations. For example, the Euler equations

$$\begin{cases} \partial_\tau \rho + \operatorname{div}(\rho v) = 0, \\ \partial_\tau v + (v \cdot \nabla)v + \frac{1}{\rho} \nabla(\rho T) = 0, \\ \partial_\tau T + (v \cdot \nabla)T + \frac{2}{3} T \nabla_x \cdot v = 0, \end{cases}$$

or the incompressible Navier-Stokes equations

$$\partial_\tau v + (v \cdot \nabla)v = -\nabla p + \nu \Delta v \quad \text{with} \quad \nabla_x \cdot v = 0,$$

in the latter case,  $p$  stands for the pressure which is determined by the incompressibility constraint.

At the microscopic scale, a gas is made of atoms whose coordinates  $\{(x_i(t), v_i(t))\}_{i \leq N}$  evolve in time according to Newtonian dynamics

$$\frac{dx_i}{dt} = v_i, \quad m \frac{dv_i}{dt} = -\frac{1}{\varepsilon} \sum_{j \neq i} \nabla \Phi \left( \frac{x_i - x_j}{\varepsilon} \right). \quad (1.8)$$

These equations are the Hamiltonian equations associated with the kinetic energy (1.1) and the potential energy (1.3). The Gibbs measure (2.18) is no longer relevant to describe the atom statistics which are now given by the evolution of a random initial data transported by the Hamiltonian flow (1.8). The macroscopic parameters  $(\rho, v, T)$  are related to the microscopic variables by local averaging, however the scaling limit is much more complicated than the thermodynamic limit (1.7) as it depends now on the space and time scales. In fact, the limiting hydrodynamic equations depend on the choice of the scaling and this explain why a fluid can be either modelled by the Euler or the Navier-Stokes equations. There is currently no mathematical derivation of the hydrodynamic equations from a purely deterministic dynamics. However by adding noise to the microscopic dynamics, the Euler equation has been obtained in [29] and the incompressible Navier-Stokes equation was derived in [32] for a class of stochastic particle systems on the cubic lattice.

Kinetic theory is a different perspective on the derivation of the hydrodynamic limits which describes the particle evolution at an intermediate scale, namely the mesoscopic scale. During a macroscopic time, each atom interacts, via the Hamiltonian flow (1.8), with a huge number of other atoms leading to intricate microscopic correlations between the atoms. Mathematically, it is then extremely difficult to recover the macroscopic parameters by averaging out microscopic coordinates with such a complex correlation structure. Kinetic theory describes the system at the mesoscopic scale defined such that typically, an atom encounters only a finite number of collisions. This corresponds to a dilute gas regime with rare collisions. At the mesoscopic scale, the system can be reduced to a probability density  $f(t, x, v)$  which records the probability of finding, at time  $t$ , an atom at position  $x$  with velocity  $v$ . This density evolves according to the Boltzmann equation

$$\begin{aligned} \partial_t f + v \cdot \nabla_x f &= Q(f, f), \\ Q(f, f)(x, v) &:= \int_{S^2 \times \mathbb{R}^3} \left( f(x, v') f(x, v'_2) - f(x, v) f(x, v_2) \right) b(v_2 - v, v) dv_2 dv, \end{aligned} \quad (1.9)$$

where  $v$  is a unit vector in  $\mathbb{R}^3$  and

$$v' = v - ((v - v_2) \cdot v) v, \quad v'_2 = v_2 + ((v - v_2) \cdot v) v.$$

The precise definition of the mesoscopic scaling as well as the heuristic explanation of the Boltzmann equation are postponed to Section 2.2. Compared to the macroscopic field  $(\rho, v, T)$ , the kinetic theory provides a more detailed description of the system and the macroscopic parameters are deduced by averaging with respect to the velocity

$$\begin{aligned} \rho(t, x) &= \int_{\mathbb{R}^d} f(t, x, v) dv, \quad u(t, x) = \frac{1}{\rho(t, x)} \int_{\mathbb{R}^d} v f(t, x, v) dv, \\ T(t, x) &= \frac{1}{2\rho(t, x)} \left( \int_{\mathbb{R}^d} v^2 f(t, x, v) dv - \left( \int_{\mathbb{R}^d} v f(t, x, v) dv \right)^2 \right). \end{aligned}$$

As a consequence, the fluid hydrodynamic equations can then be recovered by rescaling the Boltzmann equation (see Figure 1.3). These limits, known as the *fast relaxation limits*, are well understood mathematically and we refer the reader to the book [37] for a survey.



To perform the fast relaxation limit, the Boltzmann equation has to be rescaled on large time scales. However the convergence to the Boltzmann equation has been only proven for short time scales so that an important step is currently missing in order to complete the program of kinetic theory and to justify fully the hydrodynamic equations.

## 1.4 Overview of these notes

In the first part of these notes, the set-up of the kinetic theory is introduced (see Chapter 2) and the Boltzmann equation is derived as the limit of deterministic microscopic dynamics (see Chapter 3). This derivation raises fundamental physical questions because the microscopic evolution is reversible but the limiting kinetic equation is irreversible. This paradox will be solved, in Chapter 3, by a detailed analysis of the propagation of chaos.

The second part of these notes is devoted to the study of the particle dynamics at large times in perturbative regimes. In Chapter 4, we consider a gas at equilibrium and show that the motion of a tagged particle, in this a gas, converges in the kinetic limit to a Brownian motion. This shows that a random process can be obtained as a limit of deterministic dynamics. The corresponding hydrodynamic equation, namely the heat equation, can be derived directly from the particle system. In Chapter ??, we consider the fluctuation field in equilibrium and show that its time correlations decay according to the linearized Boltzmann equation. As a consequence of the derivation of the linearized Boltzmann equation, another linear hydrodynamic equation, namely the linear acoustic equations, can be obtained from the Hamiltonian dynamics.



# Chapter 2

## Hard-sphere dynamics

### 2.1 Microscopic description

#### 2.1.1 Definition of hard-sphere dynamics

Hard-sphere dynamics are simply billiard dynamics where the atoms are modelled as balls moving in straight line and undergoing elastic collisions. The number  $N$  of balls in the dynamics is larger than in a standard billiard game, say that  $N$  is of the order of the Avogadro number  $10^{23}$ . The billiard table is identified as the periodic domain  $\mathbb{T}^d = [0, 1]^d$  with dimension  $d \geq 2$ . Each particle has a label in  $\{1, \dots, N\}$ . Particle  $i$  is a ball of diameter  $\varepsilon > 0$  centered at  $x_i \in \mathbb{T}^d$  with velocity  $v_i \in \mathbb{R}^d$ . The coordinates of particle  $i$  are denoted by  $z_i = (x_i, v_i)$ . These balls are not allowed to overlap, so that the coordinates  $Z_N = \{z_1, z_2, \dots, z_N\}$  of a configuration with  $N$  particles are restricted to the *phase space*, i.e. to the domain

$$\mathbb{D}_\varepsilon^N := \left\{ Z_N = (X_N, V_N) \in \mathbb{T}^{dN} \times \mathbb{R}^{dN}, \quad \forall i \neq j, \quad |x_i - x_j| > \varepsilon \right\}, \quad (2.1)$$

with the notation  $X_N = \{x_1, x_2, \dots, x_N\}$  and  $V_N = \{v_1, v_2, \dots, v_N\}$ . In the following, we will always consider  $\varepsilon^d \ll \frac{1}{N}$  so that the phase space is not empty.

In dimension  $d = 1$ , the particles cannot cross and the dynamics is well understood [39, 13]. Nevertheless, very challenging questions remain if the particles have different masses. We refer to [41, 42] for an account of the open problems for one-dimensional systems. Throughout these notes, we will focus on the case  $d \geq 2$ .

For an initial configuration  $Z_N(0)$  in the domain  $\mathbb{D}_\varepsilon^N$ , the exclusion constraint between the balls holds at any time and the microscopic evolution (1.8) can be reformulated as follows: for all  $i \leq N$

$$\partial_t x_i(t) = v_i(t), \quad \partial_t v_i(t) = 0, \quad \text{if } |x_i(t) - x_j(t)| > \varepsilon \quad \text{for all } j \neq i, \quad (2.2)$$

with elastic reflection at collisions between two particles. In this case, if particles  $i, j$  with velocities  $v_i, v_j$  collide at time  $t$ , i.e.  $|x_i(t) - x_j(t)| = \varepsilon$ , then the outgoing velocities  $v'_i, v'_j$  are given by

$$\begin{cases} v'_i = v_i - ((v_i - v_j) \cdot \nu) \nu, \\ v'_j = v_j + ((v_i - v_j) \cdot \nu) \nu, \end{cases} \quad (2.3)$$

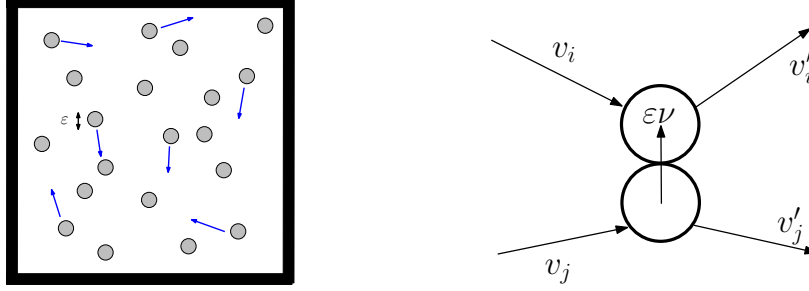


Figure 2.1: On the left, a gas with hard spheres of diameter  $\varepsilon$ . On the right, a collision between particles  $i, j$  is depicted with the notation (2.3).

where  $\nu$  is the unit vector such that  $x_i(t) = x_j(t) + \varepsilon\nu$  (see Figure 2.1). The conservation laws of the dynamics are :

$$\begin{cases} \text{Momentum conservation:} & v'_i + v'_j = v_i + v_j, \\ \text{Energy conservation:} & v_i'^2 + v_j'^2 = v_i^2 + v_j^2. \end{cases} \quad (2.4)$$

Collisions occur on configurations at the boundary  $\partial\mathbb{D}_\varepsilon^N$  of the phase space  $\mathbb{D}_\varepsilon^N$  (2.1). At a collision between particles  $i, j$ , we distinguish the pre-collisional configurations with incoming velocities

$$\begin{aligned} \partial\mathbb{D}_\varepsilon^{N-}(i, j) := \left\{ Z_N \in \partial\mathbb{D}_\varepsilon^N, \quad |x_i - x_j| = \varepsilon, \quad (v_i - v_j) \cdot (x_i - x_j) < 0 \right. \\ \left. \text{and } \forall (k, \ell) \neq (i, j), \quad |x_k - x_\ell| > \varepsilon \right\}, \end{aligned}$$

from the post-collisional configurations with outgoing velocities

$$\begin{aligned} \partial\mathbb{D}_\varepsilon^{N+}(i, j) := \left\{ Z_N \in \partial\mathbb{D}_\varepsilon^N, \quad |x_i - x_j| = \varepsilon, \quad (v_i - v_j) \cdot (x_i - x_j) > 0 \right. \\ \left. \text{and } \forall (k, \ell) \neq (i, j), \quad |x_k - x_\ell| > \varepsilon \right\}. \end{aligned}$$

Using notation (2.3), we introduce the map

$$\mathcal{J} : (v_i, v_j, \nu) \mapsto (v'_i, v'_j, -\nu) \quad (2.5)$$

which is an involution  $\mathcal{J} \circ \mathcal{J} = Id$ . From this property, we deduce that  $\mathcal{J}$  preserves the Lebesgue measure in  $\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1}$ , where  $\mathbb{S}^{d-1}$  denotes the unit ball.

Let  $\mathcal{R}$  be the map on  $\mathbb{D}_\varepsilon^N$  which reverses the velocities

$$\mathcal{R}(Z_N) = (x_1, \dots, x_N, -v_1, \dots, -v_N) \quad \text{with } Z_N = (x_1, \dots, x_N, v_1, \dots, v_N).$$

For any time  $t \geq 0$ , we denote by  $\mathbf{T}_t$  the map of the flow at time  $t$  so that for an initial data  $Z_N$  in  $\mathbb{D}_\varepsilon^N$

$$\mathbf{T}_t(Z_N) = Z_N(t). \quad (2.6)$$

A more accurate definition of  $\mathbf{T}$  is given in Proposition 2.1. Given a configuration  $Z_N(t)$  at time  $t$ , the inverse map can be obtained easily by running the dynamics backward, i.e.

by applying  $\mathbf{T}_t$  to the configuration with reversed velocities  $\mathcal{R}(Z_N(t))$  (and reversing the velocities at the final step to recover the initial data). As a consequence, the following identity holds

$$\mathbf{T}_t \mathcal{R} \mathbf{T}_t = \mathcal{R}.$$

Thus the evolution can always be traced back and there is no loss of information by the dynamics. This amounts to say that the hard-sphere flow is *time reversible*. The inverse of  $\mathbf{T}_t$  is denoted by  $\mathbf{T}_{-t}$ .

The particles interact only when they collide so that the corresponding interaction potential is degenerate

$$\Phi(r) = \begin{cases} \infty, & \text{if } r < \varepsilon, \\ 0, & \text{if } r \geq \varepsilon, \end{cases} \quad (2.7)$$

and the Hamiltonian of a configuration  $Z_N$  in  $\mathbb{D}_\varepsilon^N$  depends only on the kinetic energy

$$H_N(Z_N) := \frac{1}{2} \sum_{i=1}^N |v_i|^2. \quad (2.8)$$

By (2.4), it is a conserved quantity for the dynamics. In particular, the sets of bounded energy

$$\forall R > 0, \quad \mathbb{D}_\varepsilon^{N,R} = \left\{ Z_N \in \mathbb{D}_\varepsilon^N, \quad H_N(Z_N) \leq R^2 \right\}, \quad (2.9)$$

are invariant by the dynamics.

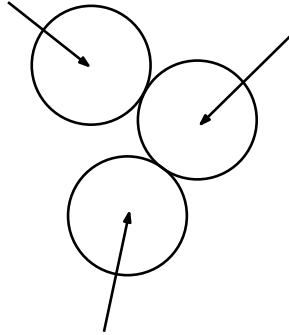


Figure 2.2: The hard-sphere flow is not well defined if 3 or more particles collide at the same time. However triple collisions never occur for almost all initial configurations.

As the potential (2.7) is degenerate the relation with (1.8) is not straightforward. In fact, the hard-sphere flow is not well defined for all initial data in  $\mathbb{D}_\varepsilon^N$ . For example, there is no dynamical rule to take into account the simultaneous collision of 3 particles (see Figure 2.2). However, the following proposition ensures that for almost all initial data (with respect to the Lebesgue measure in  $\mathbb{D}_\varepsilon^N$ ), the hard-sphere flow is well defined at any time.

**Proposition 2.1.** *The hard-sphere flow is well defined for almost all configurations in  $\mathbb{D}_\varepsilon^N$ . Furthermore outside a set of measure 0, the map  $\mathbf{T}$ , introduced in (2.6), is a one parameter group defined for all  $t \in \mathbb{R}$  which preserves Lebesgue measure.*

This result has been first proved by Alexander [4], see also [11, 15]. The singularity of the hard-sphere dynamics is a serious technical drawback to prove the kinetic limit. However the microscopic collisions in the hard-sphere dynamics have a structure very similar to the collisions in the Boltzmann equation (see (2.41)) and this will greatly simplify the derivation of the convergence to the Boltzmann equation in Chapter 3.

*Proof.* To define the hard-sphere flow, we have to exclude the pathological configurations leading to one of the following events :

- simultaneous collisions of 3 or more particles,
- grazing collisions, i.e. collisions such that  $(v_i - v_j) \cdot v = 0$  (with notation (2.3)),
- clustering, i.e. infinite number of collisions in a finite time.

Our goal is to build a dense open subset in  $\mathbb{D}_\varepsilon^N$  consisting of configurations with only finitely many (pairwise) collisions in any time interval  $[0, T]$ , so that any of the previous events will be excluded.

On a given time interval  $[0, T]$ , we are going to show that the flow is well defined on the set  $\mathbb{D}_\varepsilon^{N,R}$  of configurations with bounded energy (2.9) outside a set  $\mathcal{S}_{T,R}$  of zero measure. Then taking diverging sequences of times  $T_n$  and energy cut-off  $R_n$ , the dynamics can be defined in  $\mathbb{D}_\varepsilon^N$  for any time and any initial data outside the set  $\bigcup_n \mathcal{S}_{T_n, R_n}$  of measure zero.

We split  $[0, T]$  into small time intervals of size  $\delta > 0$  and consider the set

$$\mathbf{P}_\delta = \left\{ Z_N \in \mathbb{D}_\varepsilon^{N,R}, \text{ a particle collides twice during the time interval } [0, \delta] \right. \quad (2.10)$$

$$\left. \text{or has a grazing collision} \right\}.$$

During  $[0, \delta]$ , the flow is well defined outside the set  $\mathbf{P}_\delta$  as each particle undergoes at most one collision. For any time  $t \in [0, \delta]$ , the mapping  $\mathbf{T}_t$  is well defined in the complement of  $\mathbf{P}_\delta$  which turns out to be an open set. Furthermore, any initial data in  $\mathbf{P}_\delta^c$  leads to a trajectory with a finite number of distinct collisions which depends smoothly on the initial data. We stress the fact that the configurations with grazing collisions have been neglected as the trajectories are not smooth in their vicinity. The mapping  $\mathbf{T}_t$  is a diffeomorphism which leaves Lebesgue measure invariant. This latter point can be checked as the free flow (2.2) and the reflections (2.3) have both Jacobian equal to 1 (see [3] for details).

We are going to show that the measure of  $\mathbf{P}_\delta$  is bounded from above by

$$|\mathbf{P}_\delta| = \int_{\mathbf{P}_\delta} dZ_N \leq C\delta^2, \quad (2.11)$$

where the constant  $C$  depends on  $R, N, \varepsilon$ . Suppose that particle  $i$  collides with the two particles  $j, k$  in a time smaller than  $\delta$ . As the velocities are all bounded by  $R$ , the particles  $j, k$  have to be close to particle  $i$  initially

$$\varepsilon \leq |x_i - x_j| \leq \varepsilon + 2R\delta \quad \text{and} \quad \varepsilon \leq |x_i - x_k| \leq \varepsilon + 2R\delta,$$

where the lower bound is due to the hard-sphere constraint. The factor  $\delta^2$  in (2.11) comes from the integration with respect to  $dx_j dx_k$  as both particles  $j, k$  are located in a shell of width  $2R\delta$  around the ball  $i$  :

$$\forall x_i \in \mathbb{T}^d, \quad \int dx_j dx_k \mathbf{1}_{\{\varepsilon \leq |x_i - x_j| \leq \varepsilon + 2R\delta\}} \mathbf{1}_{\{\varepsilon \leq |x_i - x_k| \leq \varepsilon + 2R\delta\}} \leq (cR\varepsilon^{d-1}\delta)^2,$$

The remaining variables in (2.11) are then integrated and the integral is estimated by the crude upper bound  $C$ .

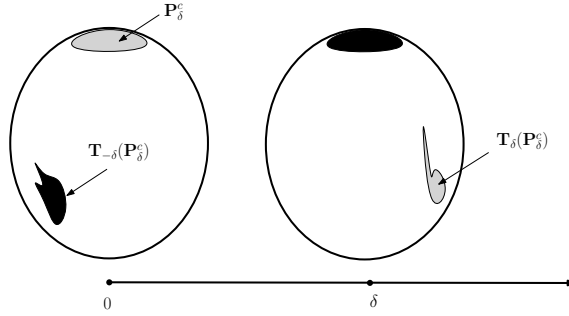


Figure 2.3: The phase space  $\mathbb{D}_\varepsilon^{N,R}$  is schematically represented by an ellipse. At time 0, the subset  $\mathbf{P}_\delta$  of configurations (represented in gray) is removed from  $\mathbb{D}_\varepsilon^{N,R}$ . At the later time  $\delta$ , the subset  $\mathbf{T}_\delta(\mathbf{P}_\delta^c) \cap \mathbf{P}_\delta \subset \mathbf{P}_\delta$  of configurations (represented in black) is removed again. This boils down to remove its pre-image  $\mathbf{P}_\delta^{(1)} = \mathbf{T}_{-\delta}(\mathbf{T}_\delta(\mathbf{P}_\delta^c) \cap \mathbf{P}_\delta)$  at time 0. The flow can be constructed up to time  $T$  by removing subsets of the phase space at each time step  $\delta$ .

The flow is well defined up to time  $\delta$  for initial data in  $\mathbf{P}_\delta^c$  and the configurations are mapped to the set  $\mathbf{T}_\delta(\mathbf{P}_\delta^c)$  at time  $\delta$ . To extend the dynamics on  $[\delta, 2\delta]$ , we consider only the configurations at time  $\delta$  for which each particle undergoes at most one collision in  $[\delta, 2\delta]$ , i.e. that the configurations in the set  $\hat{\mathbf{P}}_\delta^{(1)} = \mathbf{T}_\delta(\mathbf{P}_\delta^c) \cap \mathbf{P}_\delta$  at time  $\delta$  are discarded. This amounts to neglecting also the initial configurations in  $\mathbf{P}_\delta^{(1)} = \mathbf{T}_{-\delta}(\hat{\mathbf{P}}_\delta^{(1)})$ . As the mapping  $\mathbf{T}$  leaves Lebesgue measure invariant, the measure of  $\mathbf{P}_\delta^{(1)}$  will be less than  $C\delta^2$  thanks to (2.11). For any initial data outside the set  $\mathbf{P}_\delta \cup \mathbf{P}_\delta^{(1)}$ , the dynamics is well defined up to time  $2\delta$ . One can then iterate this procedure and extend the flow on the interval  $[k\delta, (k+1)\delta]$  by removing sets of initial configurations of the form  $\mathbf{P}_\delta^{(k)}$  with measure less than  $C\delta^2$ . Splitting the time  $T$  into  $K = \frac{T}{\delta}$  time intervals, the dynamics can be defined up to time  $T$  for initial configurations outside the set

$$\mathbf{P}_\delta(T, R) = \mathbf{P}_\delta \cup \mathbf{P}_\delta^{(1)} \cup \dots \cup \mathbf{P}_\delta^{(K)}$$

which has a measure bounded by

$$|\mathbf{P}_\delta(T, R)| \leq (K+1)C\delta^2 \leq 2CT\delta.$$

The sets associated with the sequence  $\delta_k = 2^{-k}$  are decreasing

$$\mathbf{P}_{\delta_{k+1}}(T, R) \subset \mathbf{P}_{\delta_k}(T, R).$$

Thus the set  $\bigcap_k \mathbf{P}_{\delta_k}(T, R)$  has measure 0 and the flow is well defined outside this set.  $\square$

### 2.1.2 Liouville equation

We have seen in Proposition 2.1 that the hard-sphere flow is only defined for almost all initial configurations. From a physical point of view, this is not a serious issue, as the detailed description of a single configuration trajectory is irrelevant. The main goal is to model the statistical properties of the gas and therefore we will focus on the evolution of the probability measures on the configurations.

Initially the configurations  $Z_N$  are distributed in  $\mathbb{D}_\varepsilon^N$  according to the density  $f_N(0, Z_N)$  such that

$$\int_{\mathbb{T}^{dN} \times \mathbb{R}^{dN}} dX_N dV_N f_N(0, Z_N) = 1,$$

where  $dX_N$  stands for the Lebesgue measure  $dx_1 \dots dx_N$  in  $\mathbb{T}^{dN}$  and  $dV_N$  stands for the Lebesgue measure  $dv_1 \dots dv_N$  in  $\mathbb{R}^{dN}$ . We will also use the notation  $dZ_N = dX_N dV_N$ . All the particles should behave in the same way, so that we will consider initial measures which are symmetric with respect to the particle labels. This symmetry will be preserved at any time.

According to Proposition 2.1, for almost all initial data  $Z_N$ , the configuration  $Z_N(t) = \mathbf{T}_t(Z_N)$ , at time  $t$ , is obtained by the mapping  $\mathbf{T}_t$  defined in (2.6). Thus the particle density at time  $t$  is the image of the density at time 0 by the mapping  $\mathbf{T}_t$

$$f_N(t, Z_N) = f_N(0, \mathbf{T}_{-t}Z_N). \quad (2.12)$$

To rephrase this relation in simpler terms, we suppose for a moment that  $N = 1$  and we consider the evolution of a single particle  $z_1(t)$ . The particle moves in straight line according to

$$\forall t \geq 0, \quad x_1(t) = x_1 + v_1 t, \quad v_1(t) = v_1, \quad (2.13)$$

where the coordinates of  $x_1(t)$  should be understood modulo 1 so that the configuration remains in the periodic domain  $\mathbb{T}^d$ . Then the relation (2.12) reads

$$f_1(t, x_1, v_1) = f_1(0, x_1 - v_1 t, v_1).$$

Taking the time derivative, we see that the distribution obeys the transport equation

$$\partial_t f_1(t, x_1, v_1) = -v_1 \cdot \nabla_{x_1} f_1(0, x_1 - v_1 t, v_1) = -v_1 \cdot \nabla_{x_1} f_1(t, x_1, v_1),$$

where we used the notation

$$w \cdot \nabla_x \varphi = \sum_{k=1}^d w_k \partial_k \varphi \quad \text{with} \quad w = (w_1, \dots, w_d) \in \mathbb{R}^d$$

and  $\partial_k$  is the derivative with respect to the  $k^{\text{th}}$ -coordinate of  $x \in \mathbb{T}^d$ .

A similar computation holds also for a hard-sphere gas with  $N$  particles since the particles do not interact in between two collisions. Thus the density satisfies the *Liouville equation* in  $\mathbb{D}_\varepsilon^N$

$$\partial_t f_N(t, Z_N) + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f_N(t, Z_N) = 0. \quad (2.14)$$



However, one has also to prescribe boundary conditions on the density in  $\partial\mathbb{D}_\varepsilon^N$  to take into account the collisions. We impose that on each set  $\partial\mathbb{D}_\varepsilon^{N+}(i, j)$  of post-collisional configurations the density is given by

$$f_N(t, Z'_N) = f_N(t, Z_N), \quad (2.15)$$

where  $Z'_N$  is obtained from the configuration  $Z_N \in \partial\mathbb{D}_\varepsilon^{N-}(i, j)$  by changing the velocities  $v_i, v_j$  into  $v'_i, v'_j$  according to the collision rule (2.3). Finally, we define  $\mathbf{S}_N$  the group associated with the transport in  $\mathbb{D}_\varepsilon^N$  by

$$\forall \varphi \in \mathbb{L}^\infty(\mathbb{D}_\varepsilon^N), \quad \mathbf{S}_N(t)\varphi : Z_N \mapsto \varphi(\mathbf{T}_{-t}(Z_N)). \quad (2.16)$$

In particular, the density at time  $t$  defined in (2.12) can be rewritten

$$f_N(t, Z_N) = \left( \mathbf{S}_N(t) f_N(0) \right) (Z_N).$$

So far the Liouville equation was interpreted as the evolution equation for probability measures, but it can be solved for more general initial data. The following proposition will be used, later on, to derive uniform estimates on the density of the hard-sphere dynamics.

**Proposition 2.2** (Maximum principle). *Let  $g_N, h_N$  be two solutions of the Liouville equation with initial data such that  $g_N(0, Z_N) \leq h_N(0, Z_N)$  for almost all configuration  $Z_N$  in  $\mathbb{D}_\varepsilon^N$ , then the order is preserved at any time  $t \geq 0$*

$$g_N(t, Z_N) \leq h_N(t, Z_N),$$

for almost all configuration in  $Z_N \in \mathbb{D}_\varepsilon^N$ .

*Proof.* Thanks to (2.12), the solutions at time  $t$  can be expressed in terms of the initial data

$$h_N(t, Z_N) - g_N(t, Z_N) = h_N(0, \mathbf{T}_{-t}Z_N) - g_N(0, \mathbf{T}_{-t}Z_N) \geq 0.$$

This completes Proposition 2.2. □

### 2.1.3 Invariant measures

Before studying the evolution of the particle density, we are going to focus on the stationary solutions of the Liouville equation (2.14) which will play a key role in these notes. For  $s \geq 1$  and  $\beta > 0$ , the Maxwellian distribution in  $\mathbb{R}^{ds}$  is denoted by

$$M_\beta^{\otimes s}(V_s) := \prod_{i=1}^s M_\beta(v_i) \quad \text{with} \quad M_\beta(v) := \left( \frac{\beta}{2\pi} \right)^{\frac{d}{2}} \exp\left( -\frac{\beta}{2}|v|^2 \right). \quad (2.17)$$

In physics, the parameter  $\beta$  is interpreted as the inverse of a temperature. The *Gibbs measure* on the particle configurations in  $\mathbb{T}^{dN} \times \mathbb{R}^{dN}$  is defined by

$$M_{N,\beta}(Z_N) := \frac{1}{\mathcal{Z}_N} \left( \frac{\beta}{2\pi} \right)^{\frac{dN}{2}} \exp(-\beta H_N(V_N)) \mathbf{1}_{\mathbb{D}_\varepsilon^N}(Z_N) = \frac{1}{\mathcal{Z}_N} \mathbf{1}_{\mathbb{D}_\varepsilon^N}(Z_N) M_\beta^{\otimes N}(V_N), \quad (2.18)$$

where the Hamiltonian  $H_N$  was introduced in (2.8) and the partition function  $\mathcal{Z}_N$  is the normalization factor

$$\mathcal{Z}_N := \int_{\mathbb{T}^{dN} \times \mathbb{R}^{dN}} \mathbf{1}_{\mathbb{D}_\varepsilon^N}(Z_N) M_\beta^{\otimes N}(V_N) dZ_N = \int_{\mathbb{T}^{dN}} \prod_{1 \leq i \neq j \leq N} \mathbf{1}_{|x_i - x_j| > \varepsilon} dX_N. \quad (2.19)$$

Under the Gibbs measure, only the positions are correlated by the exclusion constraint between the particles. We stress the fact that the particles play a symmetric role so that the measure is *exchangeable*.

**Proposition 2.3.** *The Gibbs measure  $M_{N,\beta}$  is an invariant measure for the gas dynamics.*

*Proof.* The Gibbs measure is a solution of the Liouville equation (2.14) as it is constant in time and with respect to the positions of the configurations in  $\mathbb{D}_\varepsilon^N$ . Furthermore the boundary conditions (2.15) are satisfied thanks to the conservation of the kinetic energy (2.4) by the elastic collisions.  $\square$

Under the Gibbs measure the positions of the particles are uniformly distributed in the set  $\{X_N, \ i \neq j, \ |x_i - x_j| \geq \varepsilon\}$ . The effect of the exclusion strongly depends on the particle density

$$\rho := N\kappa_d \varepsilon^d, \quad (2.20)$$

where  $\kappa_d \varepsilon^d$  stands for the volume of a particle. At large density, the correlations between the particles are so strong that physicists expect the occurrence of a phase transition [1, 44]. This has been observed numerically, but there is no mathematical proof of it yet. The behavior of the Gibbs measure is much simpler at low density. Indeed when the diameter  $\varepsilon$  of the particles tends to 0, the exclusion constraint between the particles becomes less relevant. At  $\varepsilon = 0$ , the positions are independent and uniformly distributed in  $\mathbb{T}^{dN}$  under the measure  $M_{N,\beta}$  as there is no interaction. Thus we expect that for  $\rho$  small enough, the Gibbs measure behaves as a perturbation of the product measure.

To quantify the properties of the Gibbs measure  $M_{N,\beta}$ , we define for any fixed  $s \geq 1$ , the marginal of order  $s$  by

$$M_{N,\beta}^{(s)}(Z_s) := \int M_{N,\beta}(Z_N) dz_{s+1} \dots dz_N. \quad (2.21)$$

If the particles were not interacting then the measure  $M_{N,\beta}^{(s)}$  would be equal to the Gibbs measure  $M_{s,\beta}$ . The following proposition shows that both measures remain close at very low density, in particular the particles become asymptotically independent when  $\rho \rightarrow 0$ . Note that  $M_{s,\beta}$  is equal to the measure  $M_\beta^{\otimes s} \mathbf{1}_{\mathbb{D}_\varepsilon^s}$  up to the normalization factor  $\mathcal{Z}_s$ .

**Proposition 2.4.** *Given  $\beta > 0$ , there is a constant  $C > 0$  such that for any  $\rho \leq 1/2$  the following bound holds uniformly in  $N$  and  $s \leq N$ .*

$$\left| \left( M_{N,\beta}^{(s)} - M_\beta^{\otimes s} \right) \mathbf{1}_{\mathbb{D}_\varepsilon^s} \right| \leq C^s \rho M_\beta^{\otimes s}. \quad (2.22)$$

Better estimates can be obtained and we refer the reader to [36] for a detail account.

*Proof.*

**Step 1.** We are going to derive the following estimate on the partition function (2.19)

$$\forall s \leq N, \quad 1 \leq \frac{\mathcal{Z}_{N-s}}{\mathcal{Z}_N} \leq (1 - \rho)^{-s}. \quad (2.23)$$

The first inequality follows by removing the exclusion constraint on the last  $s$  particles

$$\mathcal{Z}_N \leq \mathcal{Z}_{N-s}.$$

Let us prove the second inequality in (2.23). Recall that

$$\mathcal{Z}_{s+1} = \int_{\mathbb{T}^{d(s+1)}} \left( \prod_{1 \leq i \neq j \leq s+1} \mathbf{1}_{|x_i - x_j| > \varepsilon} \right) dX_{s+1}.$$

By Fubini's theorem, we deduce that

$$\mathcal{Z}_{s+1} = \int_{\mathbb{T}^{ds}} \left( \int_{\mathbb{T}^d} \left( \prod_{1 \leq i \leq s} \mathbf{1}_{|x_i - x_{s+1}| > \varepsilon} \right) dx_{s+1} \right) \left( \prod_{1 \leq i \neq j \leq s} \mathbf{1}_{|x_i - x_j| > \varepsilon} \right) dX_s.$$

Since the volume excluded by the  $s$  particles is at most  $s\kappa_d \varepsilon^d$ , we get

$$\int_{\mathbb{T}^d} \left( \prod_{1 \leq i \leq s} \mathbf{1}_{|x_i - x_{s+1}| > \varepsilon} \right) dx_{s+1} \geq 1 - s\kappa_d \varepsilon^d,$$

where  $\kappa_d \varepsilon^d$  stands for the volume of one particle. This implies the lower bound

$$\mathcal{Z}_{s+1} \geq \mathcal{Z}_s (1 - s\kappa_d \varepsilon^d) \geq \mathcal{Z}_s (1 - \rho),$$

where we used  $s \leq N$  and  $\rho = N\kappa_d \varepsilon^d$ . Inequality (2.23) is then completed by induction

$$\mathcal{Z}_N \geq \mathcal{Z}_{N-s} (1 - \rho)^s.$$

**Step 2.** We derive now Inequality (2.44). For  $s \leq N$ , the marginal is given by

$$\begin{aligned} M_{N,\beta}^{(s)}(Z_s) &= \frac{1}{\mathcal{Z}_N} \mathbf{1}_{\{Z_s \in \mathbb{D}_\varepsilon^s\}} M_\beta^{\otimes s}(V_s) \int_{\mathbb{R}^{d(N-s)}} M_\beta^{\otimes (N-s)}(V_{s+1,N}) dV_{s+1,N} \\ &\quad \times \int_{\mathbb{T}^{d(N-s)}} \left( \prod_{s+1 \leq k \neq \ell \leq N} \mathbf{1}_{|x_k - x_\ell| > \varepsilon} \right) \left( \prod_{i \leq s < j} \mathbf{1}_{|x_i - x_j| > \varepsilon} \right) dX_{s+1,N}, \end{aligned}$$

with the notation

$$dX_{s+1,N} := dx_{s+1} \dots dx_N \quad \text{and} \quad dV_{s+1,N} := dv_{s+1} \dots dv_N.$$

As the velocities are decoupled from the positions, the measure on the velocities factorizes. It remains to estimate the effect of the interaction between the positions of the first  $s$  particles and the rest of the system. Using the symmetry, we get that

$$M_{N,\beta}^{(s)} = \frac{1}{\mathcal{Z}_N} \mathbf{1}_{\{Z_s \in \mathbb{D}_\varepsilon^s\}} M_\beta^{\otimes s} \left( \mathcal{Z}_{N-s} - \mathcal{Z}_{(s+1,N)}^b \right) \quad (2.24)$$

with the notation

$$\mathcal{Z}_{(s+1,N)}^b := \int_{\mathbb{T}^{d(N-s)}} \left( 1 - \prod_{i \leq s < j} \mathbf{1}_{|x_i - x_j| > \varepsilon} \right) \prod_{s+1 \leq k \neq \ell \leq N} \mathbf{1}_{|x_k - x_\ell| > \varepsilon} dX_{s+1,N}.$$

This leads to the following decomposition

$$\mathbf{1}_{\{Z_s \in \mathbb{D}_\varepsilon^s\}} \left( M_\beta^{\otimes s} - M_{N,\beta}^{(s)} \right) = \left( 1 - \frac{\mathcal{Z}_{N-s}}{\mathcal{Z}_N} \right) \mathbf{1}_{\{Z_s \in \mathbb{D}_\varepsilon^s\}} M_\beta^{\otimes s} + \frac{\mathcal{Z}_{(s+1,N)}^b}{\mathcal{Z}_N} \mathbf{1}_{\{Z_s \in \mathbb{D}_\varepsilon^s\}} M_\beta^{\otimes s}. \quad (2.25)$$

Inequality (2.23) implies that there is  $C > 0$  such that for all  $\rho \leq 1/2$

$$\forall s \leq N, \quad \left| 1 - \frac{\mathcal{Z}_{N-s}}{\mathcal{Z}_N} \right| \leq (1 - \rho)^{-s} - 1 \leq C^s \rho.$$

Thus the first term in (2.25) is under control. To estimate the second term, we note that

$$0 \leq 1 - \prod_{i \leq s < j} \mathbf{1}_{|x_i - x_j| > \varepsilon} \leq \sum_{i \leq s < j} \mathbf{1}_{|x_i - x_j| < \varepsilon}$$

leads to the bound

$$\mathcal{Z}_{(s+1,N)}^b \leq \sum_{1 \leq i \leq s} \int_{\mathbb{T}^{d(N-s)}} \left( \sum_{s+1 \leq j \leq N} \mathbf{1}_{|x_i - x_j| < \varepsilon} \right) \prod_{s+1 \leq k \neq \ell \leq N} \mathbf{1}_{|x_k - x_\ell| > \varepsilon} dX_{s+1,N}.$$

Using the symmetry between the particles and Fubini's equality, we get

$$\begin{aligned} & \int_{\mathbb{T}^{d(N-s)}} \left( \sum_{s+1 \leq j \leq N} \mathbf{1}_{|x_i - x_j| < \varepsilon} \right) \prod_{s+1 \leq k \neq \ell \leq N} \mathbf{1}_{|x_k - x_\ell| > \varepsilon} dX_{s+1,N} \\ & \leq (N-s) \int_{\mathbb{T}^d} \mathbf{1}_{|x_i - x_{s+1}| < \varepsilon} dx_{s+1} \int_{\mathbb{T}^{d(N-s-1)}} \prod_{s+2 \leq k \neq \ell \leq N} \mathbf{1}_{|x_k - x_\ell| > \varepsilon} dX_{s+2,N} \\ & = (N-s) \left( \int_{\mathbb{T}^d} \mathbf{1}_{|x_i - x_{s+1}| < \varepsilon} dx_{s+1} \right) \times \mathcal{Z}_{N-s-1}, \end{aligned}$$

where, in the second inequality, the interaction between  $s+1$  and the rest of the particles has been removed and bounded from above by 1. We deduce that

$$\mathcal{Z}_{(s+1,N)}^b \leq s(N-s) \varepsilon^d \kappa_d \mathcal{Z}_{N-s-1} \leq s \rho \frac{\mathcal{Z}_{N-s-1}}{\mathcal{Z}_N} \mathcal{Z}_N \leq \frac{s}{(1-\rho)^s} \rho \mathcal{Z}_N, \quad (2.26)$$

where the last equality follows from (2.23). This shows that the second term in (2.25) is also bounded by  $C^s \rho$ , for some constant  $C$ .

The proof of Proposition 2.4 is complete.  $\square$

Before concluding this section, let us stress that the Gibbs measures  $M_{N,\beta}$  (2.18) are not the only invariant measures : as the kinetic energy is conserved, any probability distribution of the form  $F(H_N)M_{N,\beta}$  is also invariant. Nevertheless, in the large  $N$  limit, the Maxwellian turns out to be the only relevant measures for the marginal density. Indeed, for any  $\beta > 0$ , if one considers  $\mathcal{U}_N$  the uniform measure on the set of codimension 1

$$\{(V_1, \dots, V_N) \in \mathbb{R}^{dN}; \quad H_N(V_N) = \beta N\}$$

then the marginals converge to a product of Maxwellian when  $N$  tends to infinity (this result is known as Poincaré Lemma, see [26])

$$\forall s \geq 1, \quad \mathcal{U}_N^{(s)} \xrightarrow[N \rightarrow \infty]{(law)} M_\beta^{\otimes s}.$$

For this reason, it is enough to focus on the measures of the form  $M_{N,\beta}$ .

### 2.1.4 BBGKY hierarchy

To describe the coarse grained behavior of a gas, it is enough to investigate the averaged evolution of a few particles as the distribution  $f_N(t, Z_N)$ , introduced in (2.12), is symmetric with respect to all the labels. Thus for  $s < N$ , we introduce the marginal

$$f_N^{(s)}(t, Z_s) := \int f_N(t, Z_N) dz_{s+1} \dots dz_N.$$

We are going to define the analog of the Liouville equation (2.14) for the marginals. This is known as the BBGKY hierarchy. The initials stand for Bogoliubov, Born, Green, Kirkwood and Yvon who discovered this hierarchy of equations independently.

In the case  $s = 1$ , a formal computation shows that

$$\begin{aligned} & \partial_t f_N^{(1)}(t, z_1) + v_1 \cdot \nabla_{x_1} f_N^{(1)}(t, z_1) \\ &= (N-1) \varepsilon^{d-1} \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_N^{(2)}(t, x_1, v'_1, x_1 + \varepsilon v, v'_2) ((v_2 - v_1) \cdot v)_+ dv dv_2 \\ & \quad - (N-1) \varepsilon^{d-1} \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_N^{(2)}(t, x_1, v_1, x_1 + \varepsilon v, v_2) ((v_2 - v_1) \cdot v)_- dv dv_2, \end{aligned} \quad (2.27)$$

with the collision rule

$$v'_1 := v_1 - ((v_1 - v_2) \cdot v) v, \quad v'_2 := v_2 + ((v_1 - v_2) \cdot v) v. \quad (2.28)$$

Note that this collision rule is the inverse of the mapping (2.3) :  $v'_1, v'_2$  should be interpreted as incoming velocities.

Equation (2.27) says that particle 1 travels in a straight line before colliding with another of the  $(N-1)$  remaining particles. As all the particles play a symmetric role, we can assume that the collision occurs with particle 2 at position  $x_2 = x_1 + \varepsilon v$ . The contribution  $\varepsilon^{d-1}$  comes from the fact that the collision occurs at the surface of particle 1 (which is a sphere of diameter  $\varepsilon$ ). Finally in the right hand side of the equation, the gain part corresponds to a collision leading to an outgoing velocity  $v_1$ , instead the loss part is associated with a collision with an incoming velocity  $v_1$ .

Before commenting further on equation (2.27), let us stress that solving the evolution of a single particle density  $f_N^{(1)}$  requires the knowledge of the marginal  $f_N^{(2)}$  to compute the collision term. Thus we are led to write the family of equations for all the marginals which is known as the *BBGKY hierarchy*. The marginal of order  $s < N$  evolves in  $\mathbb{D}_\varepsilon^s$  according to

$$\partial_t f_N^{(s)}(t, Z_s) + \sum_{i=1}^s v_i \cdot \nabla_{x_i} f_N^{(s)}(t, Z_s) = (C_{s,s+1} f_N^{(s+1)})(t, Z_s) \quad (2.29)$$

with the boundary condition in  $\partial\mathbb{D}_\varepsilon^s$  as in (2.15)

$$f_N^{(s)}(t, Z'_s) = f_N^{(s)}(t, Z_s).$$

The structure of the collision term is similar to the source term in (2.27)

$$C_{s,s+1} = C_{s,s+1}^+ - C_{s,s+1}^-, \quad (2.30)$$

where the gain and the loss part of the operator are defined for any smooth function  $f_{s+1}$  by

$$\begin{aligned} C_{s,s+1}^+ f_{s+1}(Z_s) &= (N-s)\varepsilon^{d-1} \sum_{i=1}^s \int f_{s+1}(\dots, x_i, v'_i, \dots, x_i + \varepsilon v, v'_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_+ dv dv_{s+1}, \\ C_{s,s+1}^- f_{s+1}(Z_s) &= (N-s)\varepsilon^{d-1} \sum_{i=1}^s \int f_{s+1}(\dots, x_i, v_i, \dots, x_i + \varepsilon v, v_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_- dv dv_{s+1}. \end{aligned}$$

The hierarchy stops at  $s = N$  which coincides with Liouville equation (2.14). Thus all the informations on the dynamics are encoded at the level  $s = N$  and the other equations are simply consequences of Liouville equation. However the hierarchy will be extremely useful to describe the structure of the correlations between particles.

The collision operators (2.30) require to integrate functions on sets of codimension 1, i.e. on the surface of a particle. The flow is defined only for almost all initial data (see Proposition 2.1), thus the measure  $f_N$  and the marginals  $f_N^{(s)}$  are also defined almost surely. This lack of regularity means that the equations (2.29) of the BBGKY hierarchy are formal. To make sense of these equations, they need to be rewritten in the mild sense. This has been achieved in [38, 15, 31, 11]. Below, we will follow an approach inspired by [38, 31].

Recall that for any integer  $s$ , the group  $\mathbf{S}_s$  associated with the transport in  $\mathbb{D}_\varepsilon^s$  was defined in (2.16) as

$$\forall \varphi \in \mathbb{L}^\infty(\mathbb{D}_\varepsilon^s), \quad \mathbf{S}_s(t)\varphi : Z_s \mapsto \varphi(\mathbf{T}_{-t}(Z_s)). \quad (2.31)$$

We are going to derive a mild version of the formal equation (2.29).

**Proposition 2.5.** *Assume that the initial distribution  $f_N(0)$  is bounded from above and supported in  $\mathbb{D}_\varepsilon^{N,R}$  for some  $R$ . Then for any times  $t, \delta \geq 0$ , we get*

$$f_N^{(s)}(t + \delta) = \mathbf{S}_s(\delta) f_N^{(s)}(t) + \int_0^\delta d\tau \mathbf{S}_s(\delta - \tau) C_{s,s+1} \mathbf{S}_{s+1}(\tau) f_N^{(s+1)}(t) + O(\delta^2), \quad (2.32)$$

where the error term depends on  $N, \varepsilon, R, \|f_N(0)\|_\infty$ .

Before proving Proposition 2.5, let us first relate it to the BBGKY hierarchy. In formula (2.32), the collision operator  $C_{s,s+1}$  does not apply directly to  $f_N^{(s+1)}$  but to  $\mathbf{S}_{s+1}(\tau) f_N^{(s+1)}$

so that the additional time parameter  $\tau$  compensates the missing dimension. The role of the parameter  $\tau$  will be made more transparent in the proof below.

Equation (2.29) can be recovered by taking the time derivative (i.e. by letting  $\delta$  tend to 0 in (2.32)): the first term  $\mathbf{S}_s(\delta)$  is associated with the transport part and the second term formally converges to the collision operator applied to  $f_N^{(s+1)}(t)$ .

*Proof.* For simplicity, we choose  $t = 0$  as the proof does not depend on the structure of the initial data. In fact, the error term depends on  $\|f_N(t)\|_\infty$ , but one can deduce from Proposition 2.2 that  $\|f_N(t)\|_\infty \leq \|f_N(0)\|_\infty$  thus there is no loss of generality to consider only the case  $t = 0$ . We are going to prove (2.32) in the case  $s = 1$

$$f_N^{(1)}(\delta, z_1) = \left( \mathbf{S}_1(\delta) f_N^{(1)}(0) \right)(z_1) + \int_0^\delta d\tau \left( \mathbf{S}_1(\delta - \tau) C_{1,2} \mathbf{S}_2(\tau) f_N^{(2)}(0) \right)(z_1) + O(\delta^2). \quad (2.33)$$

The proof is split into several steps.

**Step 1.** *Decomposition of the trajectory.*

Let  $\mathbb{E}$  be the expectation of the particle trajectories starting from the initial measure  $f_N(0)$ . In particular, for any function  $\varphi$  in  $\mathbb{T}^d \times \mathbb{R}^d$ , one can write

$$\mathbb{E}(\varphi(z_1(\delta))) = \int f_N^{(1)}(\delta, z_1) \varphi(z_1) dz_1.$$

In the previous expectation, the coordinates of the other particles are averaged and their exact positions are unknown. Thus, on a short time scale, the evolution of the first particle will be very similar to a Markov chain with random kicks at random times. By analogy with a Poisson process, the expectation can be decomposed as

$$\begin{aligned} \mathbb{E}(\varphi(z_1(\delta))) &= \mathbb{E} \left( \varphi(z_1(\delta)) \mathbf{1}_{\{1 \text{ has no collisions in } [0, \delta]\}} \right) \\ &\quad + \mathbb{E} \left( \varphi(z_1(\delta)) \mathbf{1}_{\{1 \text{ has one collision in } [0, \delta]\}} \right) + O(\delta^2), \end{aligned}$$

where the error term is bounded by  $|O(\delta^2)| \leq \delta^2 C(N, \varepsilon, R) \|f_N(0)\|_\infty \|\varphi\|_1$ . This error term comes from the probability that particle 1 has more than one collision in a time  $\delta$  and it can be estimated as in the proof of Proposition 2.1. We are now going to evaluate the two other contributions independently.

**Step 2.** *Evaluating the probability of one collision during  $[0, \delta]$ .*

For any  $i \in \{2, \dots, N\}$ , let  $\mathcal{A}_i \subset \mathbb{T}^{dN} \times \mathbb{R}^{dN}$  be the set of initial configurations such that particles 1 and  $i$  collide during the time interval  $[0, \delta]$  and that they have no collision with the other particles. In the set  $\mathcal{A}_2$ , the trajectories of particles 1 and 2 are strongly constrained. Let  $z_1 = (x_1, v_1)$  be the coordinates of particle 1 at time  $\delta$  and suppose that it collides at time  $\tau \in [0, \delta]$  with particle 2 (see Figure 2.4), then the coordinates of both particles at time 0 are given by

$$\Gamma'(z_1, v_2, \tau, \nu) = \left( (x_1 - (\delta - \tau)v_1 - \tau v'_1, v'_1), (x_1 - (\delta - \tau)v_1 + \varepsilon v - \tau v'_2, v'_2) \right).$$

In this expression,  $v_1, v_2$  are outgoing velocities so that  $(v_2 - v_1) \cdot \nu > 0$  and  $v'_1, v'_2$  are the corresponding incoming velocities at time 0 given by (2.28) (see Figure 2.4). The mapping  $\Gamma'(z_1, v_2, \tau, \nu)$  is the composition of

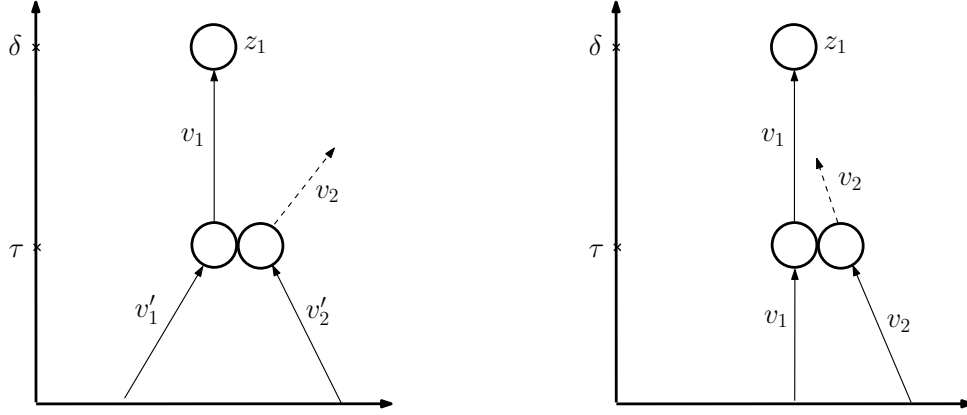


Figure 2.4: In both pictures, the vertical axis represents the time and the horizontal axis represents the space  $\mathbb{T}^d$ . Following the backward flow from the coordinate  $z_1 = (x_1, v_1)$  of the first particle at time  $\delta$ , a new particle is created at time  $\tau$ . The left picture depicts the map  $\Gamma'$  associated with the scattering, instead the right picture corresponds to the map  $\Gamma$ .

- the backward transport for the first particle during a time  $\delta - \tau$ ,
- the creation at time  $\tau$  of a new particle at position  $x_1 - (\delta - \tau)v_1 + \varepsilon v$  with velocity  $v'_2$  and the deflection of the velocity  $v_1$  into  $v'_1$ ,
- the backward transport of both particles from time  $\tau$  up to time 0.

Thus  $\Gamma'$  is defined on the set

$$\mathbf{G}^+ = \{(z_1, v_2, \tau, v) \in \mathbb{T}^d \times \mathbb{B}_R \times \mathbb{B}_R \times [0, \delta] \times \mathbf{S}^{d-1}; \quad (v_2 - v_1) \cdot v > 0\},$$

where the velocities are restricted to the set  $\mathbb{B}_R = \{v \in \mathbb{R}^d, \quad |v| \leq R\}$  as  $f_N(0)$  is supported in  $\mathbb{D}_\varepsilon^{N,R}$ . Since the velocities are bounded, the particle trajectories will not wrap around the periodic domain  $\mathbb{T}^d$  for  $\delta$  small enough so that the map  $\Gamma'$  is a bijection from  $\mathbf{G}^+$  to  $\Gamma'(\mathbf{G}^+) \subset \mathbb{T}^{2d} \times \mathbb{R}^{2d}$ . The following lemma allows us to rephrase the randomness of the initial data in terms of a random scattering of particle 1.

**Lemma 2.6.** *The change of variables  $\Gamma'$  from  $\mathbf{G}^+$  to  $\Gamma'(\mathbf{G}^+) \subset \mathbb{T}^{2d} \times \mathbb{R}^{2d}$  maps the measure  $\varepsilon^{d-1}((v_2 - v_1) \cdot v)_+ dz_1 dv_2 d\tau dv$  onto  $dz_1 dz_2$ .*

This lemma is illustrated in Figure 2.5 and its proof is postponed to the end of this section. As a consequence, the initial configuration in  $\mathcal{A}_2$  can be encoded by  $\{z_1, v_2, \tau, v, Z_{3,N}\}$  where  $Z_{3,N} = \{z_3, z_4, \dots, z_N\}$  stands for the remaining particles. Using this change of variables, we can write

$$\begin{aligned} \mathbb{E} \left( \varphi(z_1(\delta)) \mathbf{1}_{\{1 \text{ has one collision in } [0, \delta] \text{ with } 2\}} \right) &= \int dZ_N f_N(0, Z_N) \varphi(z_1(\delta)) \mathbf{1}_{\{Z_N \in \mathcal{A}_2\}} \\ &= \varepsilon^{d-1} \int ((v_2 - v_1) \cdot v)_+ dz_1 dv_2 d\tau dv \int dZ_{3,N} \mathbf{1}_{\{\Gamma'(z_1, v_2, \tau, v), Z_{3,N}\} \in \mathcal{A}_2\}} \\ &\quad \times f_N(0, \Gamma'(z_1, v_2, \tau, v), Z_{3,N}) \varphi(z_1). \end{aligned}$$

The set  $\mathcal{A}_2$  imposes two constraints on the initial data : first that particles 1 and 2 collide, second that the other particles do not collide with 1,2. Since the first constraint has been



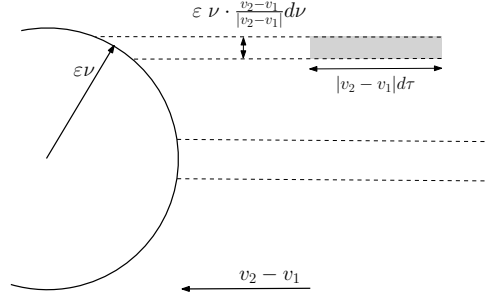


Figure 2.5: This picture illustrates the change of measure of Lemma 2.6 in dimension 2. The position  $x_2$  is parametrized by a point on the surface of the particle 1 (determined by the vector  $\varepsilon\nu$ ), the time  $\tau$  and the relative velocity  $v_2 - v_1$ . Thus a small variation of time  $d\tau$  and angle  $d\nu$  means that  $x_2$  will belong to a box of length  $|v_2 - v_1|d\tau$  and width  $\frac{(\nu \cdot (v_2 - v_1))_+}{|v_2 - v_1|}d\nu$ .

taken into account by the representation  $\Gamma'(z_1, v_2, \tau, \nu)$ , the event  $\mathcal{A}_2$  can be neglected as any further collision would lead to an event of probability of order  $\delta^2$ . Thus we get

$$\begin{aligned} & \mathbb{E}\left(\varphi(z_1(\delta))\mathbf{1}_{\{1 \text{ has one collision in } [0, \delta] \text{ with } 2\}}\right) \\ &= \varepsilon^{d-1} \int ((v_2 - v_1) \cdot \nu)_+ dz_1 dv_2 d\tau d\nu \int dZ_{3,N} f_N(0, \Gamma'(z_1, v_2, \tau, \nu), Z_{3,N}) \varphi(z_1) + O(\delta^2) \\ &= \varepsilon^{d-1} \int f_N^{(2)}(0, \Gamma'(z_1, v_2, \tau, \nu)) \varphi(z_1) ((v_2 - v_1) \cdot \nu)_+ dz_1 dv_2 d\tau d\nu + O(\delta^2), \end{aligned} \quad (2.34)$$

where the second marginal is obtained by integrating over the remaining particles. All the particles play a symmetric role, thus we deduce that

$$\begin{aligned} & \mathbb{E}\left(\varphi(z_1(\delta))\mathbf{1}_{\{1 \text{ has one collision in } [0, \delta]\}}\right) \\ &= (N-1)\varepsilon^{d-1} \int f_N^{(2)}(0, \Gamma'(z_1, v_2, \tau, \nu)) \varphi(z_1) ((v_2 - v_1) \cdot \nu)_+ dz_1 dv_2 d\tau d\nu + O(\delta^2). \end{aligned}$$

The mapping  $\Gamma'$  can be rewritten in terms of the transport operator  $\mathbf{S}_2$  and the creation operator  $C_{1,2}^+$  introduced in (2.30)

$$\begin{aligned} & \mathbb{E}\left(\varphi(z_1(\delta))\mathbf{1}_{\{1 \text{ has one collision in } [0, \delta]\}}\right) \\ &= \int dz_1 \varphi(z_1) \int_0^\delta d\tau \left( \mathbf{S}_1(\delta - \tau) C_{1,2}^+ \mathbf{S}_2(\tau) f_N^{(2)}(0) \right)(z_1) + O(\delta^2). \end{aligned} \quad (2.35)$$

This allows us to identify one of the contribution in (2.33).

**Step 3.** *Evaluating the probability of not colliding during  $[0, \delta]$ .*

We will proceed in a similar way to estimate the probability that particle 1 has no collision in  $[0, \delta]$ . Any initial data in  $\cap_{i=2}^N \mathcal{A}_i^c$  would lead to one of the following event during the time interval  $[0, \delta]$  :

- particle 1 has no collision,
- particle 1 collides more than once,

- a particle collides before colliding with 1.

The last two events involve multiple collisions in the time interval  $[0, \delta]$  and their probability can therefore be estimated from above by  $O(\delta^2)$ . Thus we can write

$$\begin{aligned}
& \mathbb{E} \left( \varphi(z_1(\delta)) \mathbf{1}_{\{1 \text{ has no collisions in } [0, \delta]\}} \right) \\
&= \int dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) \prod_{i=2}^N \left( 1 - \mathbf{1}_{\{Z_N \in \mathcal{A}_i\}} \right) + O(\delta^2) \\
&= \int dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) - \sum_{i=2}^N \int_{\mathcal{A}_i} dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) + O(\delta^2) \\
&= \int dz_1 f_N^{(1)}(0, z_1) \varphi((x_1 + \delta v_1, v_1)) - (N-1) \int_{\mathcal{A}_2} dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) + O(\delta^2),
\end{aligned}$$

where we used, in the second equality, that constraining more than one particle to hit particle 1 has a cost at least  $\delta^2$  and, in the third equality, we used the symmetry between the particles.

We are now going to change variable and parametrize the previous formula by the coordinates of particle 1 at time  $\delta$ . The first term corresponds to the free transport part in (2.33)

$$\begin{aligned}
\int dz_1 f_N^{(1)}(0, z_1) \varphi((x_1 + \delta v_1, v_1)) &= \int dz_1 f_N^{(1)}(0, (x_1 - \delta v_1, v_1)) \varphi(z_1) \\
&= \int dz_1 \varphi(z_1) \left( \mathbf{S}_1(\delta) f_N^{(1)}(0) \right)(z_1).
\end{aligned}$$

We turn now to the second term which involves  $\mathcal{A}_2$ . Let  $z_1 = (x_1, v_1)$  be the coordinates of particle 1 at time  $\delta$ , then by analogy with the mapping  $\Gamma'$ , we define

$$\Gamma(z_1, v_2, \tau, \nu) = \left( (x_1 - \delta v_1, v_1), (x_1 - (\delta - \tau)v_1 + \varepsilon v - \tau v_2, v_2) \right), \quad (2.36)$$

for configurations with incoming velocities, i.e. configurations in the set

$$\mathbf{G}^- = \left\{ (z_1, v_2, \tau, \nu) \in \mathbb{T}^d \times \mathbb{B}_R \times \mathbb{B}_R \times [0, \delta] \times \mathbb{S}^{d-1}; \quad (v_2 - v_1) \cdot \nu < 0 \right\}.$$

This map should be interpreted as the free transport for particle 1 and a direct collision between particles 1 and 2 at time  $\tau$  (see Figure 2.4). Following the proof of Lemma 2.6, one can check that  $\Gamma$  is a bijection from  $\mathbf{G}^-$  to  $\Gamma'(\mathbf{G}^-) \subset \mathbb{T}^{2d} \times \mathbb{R}^{2d}$  which maps the measure  $\varepsilon^{d-1} ((v_2 - v_1) \cdot \nu)_- dz_1 dv_2 ds dv$  onto  $dz_1 dz_2$ . Thus we can write

$$\begin{aligned}
& \int_{\mathcal{A}_2} dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) \\
&= \varepsilon^{d-1} \int ((v_2 - v_1) \cdot \nu)_- dz_1 dv_2 d\tau dv \int dZ_{3,N} \mathbf{1}_{\{(\Gamma(z_1, v_2, \tau, \nu), Z_{3,N}) \in \mathcal{A}_2\}} \\
&\quad \times f_N(0, \Gamma(z_1, v_2, \tau, \nu), Z_{3,N}) \varphi(z_1) \\
&= \varepsilon^{d-1} \int f_N^{(2)}(0, \Gamma(z_1, v_2, \tau, \nu)) \varphi(z_1) ((v_2 - v_1) \cdot \nu)_- dz_1 dv_2 d\tau dv + O(\delta^2),
\end{aligned}$$

where the restriction in  $\mathcal{A}_2$  has been removed by using the same argument as in (2.34). As in (2.35), this last term can be rewritten in terms of the collision operator

$$\begin{aligned} & (N-1) \int_{\mathcal{A}_2} dZ_N f_N(0, Z_N) \varphi((x_1 + \delta v_1, v_1)) \\ &= \int dz_1 \varphi(z_1) \int_0^\delta d\tau \left( \mathbf{S}_1(\delta - \tau) C_{1,2}^- \mathbf{S}_2(\tau) f_N^{(2)}(0) \right)(z_1) + O(\delta^2). \end{aligned}$$

This completes the derivation of (2.33) for the case  $s = 1$ .

**Step 3.** *The marginal of order  $s$ .*

The structure of formula (2.32) is similar to the one for a single particle (2.33). In a short time interval, the  $s$  particles evolve according to free transport and may collide at most once with one of the  $(N - s)$  particles in the background. Thus one would like to consider the  $s$  particles as a cloud and decompose its evolution during  $[0, \delta]$  into 3 events:

- the cloud is not impacted by background particles,
- one particle in the background collides with the cloud,
- at least two particles in the background collide with the cloud.

When implementing the previous procedure, new difficulties occur if a background particle collides successively with several of the  $s$  particles. This cannot be considered as an event of small probability because identity (2.32) holds for almost all the configurations  $Z_s$  and not only in average. These events are delicate to control and require to analyse subtle cancellations in (2.32). We refer to [38] for a complete proof.  $\square$

*Proof of Lemma 2.6.* We first derive the change of measure for the simpler map

$$\gamma(z_1, v_2, \tau, \nu) = \left( (x_1 - \tau v_1, v_1), (x_1 + \varepsilon \nu - \tau v_2, v_2) \right). \quad (2.37)$$

For simplicity, we restrict to dimension  $d = 2$  and write the coordinates as

$$x_1 = \begin{pmatrix} x_{1,1} \\ x_{1,2} \end{pmatrix}, \quad v_1 = \begin{pmatrix} v_{1,1} \\ v_{1,2} \end{pmatrix}, \quad v_2 = \begin{pmatrix} v_{2,1} \\ v_{2,2} \end{pmatrix}, \quad \nu = \begin{pmatrix} \cos(\vartheta) \\ \sin(\vartheta) \end{pmatrix}.$$

As the velocities are unchanged by  $\gamma$ , we focus on the positions

$$\begin{pmatrix} x_{1,1} + \tau v_{1,1} \\ x_{1,2} + \tau v_{1,2} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} x_{1,1} + \varepsilon \cos(\vartheta) + \tau v_{2,1} \\ x_{1,2} + \varepsilon \sin(\vartheta) + \tau v_{2,2} \end{pmatrix}. \quad (2.38)$$

The Jacobian associated with this mapping is

$$\begin{vmatrix} 1 & 0 & v_{1,1} & 0 \\ 0 & 1 & v_{1,2} & 0 \\ 1 & 0 & v_{2,1} & -\varepsilon \sin(\vartheta) \\ 0 & 1 & v_{2,2} & \varepsilon \cos(\vartheta) \end{vmatrix} = \varepsilon (\sin(\vartheta)(v_{1,2} - v_{2,2}) + \cos(\vartheta)(v_{1,1} - v_{2,1})) = \varepsilon \nu \cdot (v_1 - v_2).$$

The map  $\Gamma'$  is obtained from  $\gamma$  by composition with the free transport and then with the scattering map  $(v_1, v_2, \nu) \mapsto (v'_1, v'_2, \nu)$ . Both mappings are bijective and have unit Jacobian. This completes the derivation of Lemma 2.6 in dimension 2. A similar proof can be achieved in higher dimension leading to a surface factor  $\varepsilon^{d-1}$  instead of  $\varepsilon$ .  $\square$

## 2.2 Boltzmann-Grad limit

As explained in Section 1.3, the ultimate goal is to derive the fluid hydrodynamic equations by taking a scaling limit  $N \rightarrow \infty$  while keeping the particle density  $\rho = N\kappa_d \varepsilon^d$  of order 1. For large  $N$ , this leads to very complicated interactions between the particles and there is, so far, no mathematical derivation of the corresponding macroscopic limit (in fact the limit depends on the time and length scales at which the system is observed).

To simplify the problem, one would like to describe the statistical properties of the gas at the intermediate mesoscopic level so that a typical particle has only a finite number of collisions in a time scale of order 1. This can be achieved by considering a very dilute gas regime, i.e. by tuning  $N$  and  $\varepsilon$  according to the *Boltzmann-Grad scaling*

$$N \rightarrow \infty, \varepsilon \rightarrow 0 \quad \text{such that} \quad N\varepsilon^{d-1} = \alpha, \quad (2.39)$$

where  $\alpha > 0$  is a fixed parameter. In the Boltzmann-Grad scaling, the density  $\rho$  scales like  $\alpha\varepsilon$  and tends to 0 as  $\varepsilon$  vanishes (i.e.  $N$  when tends to infinity). A typical particle, with velocity of order 1, should collide with another particle in a time of order  $1/\alpha$ . Indeed a particle moving in a straight line during a time  $t = 1/\alpha$  will cover a cylinder of volume of order  $\varepsilon^{d-1}/\alpha$  (see Figure 2.6) and assuming that the  $N$  other particles are uniformly distributed in the domain  $\mathbb{T}^d$ , then the probability that one particle belongs to this domain is of order  $N \times \varepsilon^{d-1}/\alpha = 1$  in the Boltzmann-Grad scaling.

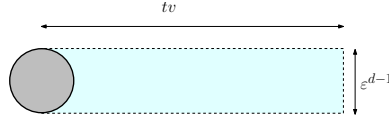


Figure 2.6: During a time  $t$ , a particle moving in a straight line covers a cylinder of volume  $tv\varepsilon^{d-1}$ .

It is expected that asymptotically, in the dilute regime, the density  $f(t, x, v)$  of a typical particle in the hard-sphere gas follows an autonomous equation known as *Boltzmann equation*

$$\begin{aligned} \partial_t f + v \cdot \nabla_x f &= \alpha Q(f, f), \\ Q(f, f)(x, v) &:= \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} \left( f(x, v') f(x, v'_2) - f(x, v) f(x, v_2) \right) b(v_2 - v, v) dv_2 dv, \end{aligned} \quad (2.40)$$

where the collision rules are the same as in (2.28)

$$v' = v - ((v - v_2) \cdot \nu) \nu, \quad v'_2 = v_2 + ((v - v_2) \cdot \nu) \nu.$$

For hard-sphere dynamics, the *cross section* is given by

$$b(v_2 - v, \nu) = ((v_2 - v) \cdot \nu)_+.$$

More general Newtonian dynamics (1.8) with an interaction potential  $\Phi$  would lead to a different cross-section  $b$ , but the structure of the collision term  $Q$  is expected to be unchanged (provided the potential  $\Phi$  decays fast enough to 0 at infinity).

Before reviewing the mathematical results on the convergence of the particle system, let us give a heuristic justification of the Boltzmann equation. The density  $f(t, x, v)$  of a typical particle should be understood as the first marginal  $f_N^{(1)}$  in the hard-sphere gas. Equation (2.27) for the evolution of this marginal is strongly reminiscent of the Boltzmann equation

$$\begin{aligned} \partial_t f_N^{(1)}(t, z_1) + v_1 \cdot \nabla_{x_1} f_N^{(1)}(t, z_1) \\ = \underbrace{(N-1)\varepsilon^{d-1}}_{\simeq \alpha} \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} \left( f_N^{(2)}(t, x_1, v'_1, x_1 + \varepsilon v, v'_2) - f_N^{(2)}(t, x_1, v_1, x_1 - \varepsilon v, v_2) \right) \\ \times ((v_2 - v_1) \cdot v)_+ dv dv_2, \end{aligned} \quad (2.41)$$

where we used the change of variable  $v \rightarrow -v$  in the loss term of the collision operator in order to factorize the cross-section. Note that the incoming particle is located at  $x_1 - \varepsilon v$  after this change of variables. The Boltzmann-Grad scaling has been precisely tuned so that the prefactor in (2.41) converges to  $\alpha$ . However, equation (2.41) keeps still a trace of the microscopic structure through the parameters  $N, \varepsilon$ . The main difficulty to recover the Boltzmann equation from (2.41) is to rewrite the marginal of order 2 in terms of  $f_N^{(1)}$ . Boltzmann's intuition was that in a very dilute gas, the particles should be almost independent and therefore the second marginal should factorize when  $\varepsilon$  is close to 0. In the article [8, 10] published in 1872, Boltzmann stated the *molecular chaos assumption*

$$\begin{aligned} f_N^{(2)}(t, x_1, v'_1, x_1 + \varepsilon v, v'_2) &\approx f_N^{(1)}(t, x_1, v'_1) f_N^{(1)}(t, x_1, v'_2), \\ f_N^{(2)}(t, x_1, v_1, x_1 - \varepsilon v, v_2) &\approx f_N^{(1)}(t, x_1, v_1) f_N^{(1)}(t, x_1, v_2), \end{aligned} \quad (2.42)$$

which formally implies the Boltzmann equation from (2.41). Note also that in the limit  $\varepsilon \rightarrow 0$ , the position of both particles are identified. In fact Boltzmann's predictions were much less quantitative than the claim (2.42) and the precise Boltzmann-Grad scaling (2.39) was formalized much later by H. Grad in [18].

The molecular chaos assumption has strong implications as it relates the microscopic and the mesoscopic levels and formally allows to encode the behavior of the gas by a single equation (2.40). In Section 2.3.1, we will see that the Boltzmann equation does not keep track of all the microscopic properties of the system and for this reason, its validity has been challenged by several physicists at the time. Starting from the work by Grad [18], many mathematicians have been working to justify rigorously the molecular chaos assumption and the convergence of the particle system towards the Boltzmann equation. We will review below some of these works.

Let us start by checking the validity of the molecular chaos assumption at time 0 for a large class of initial data. We would like to prepare the microscopic system so that each particle is sampled in  $\mathbb{T}^d \times \mathbb{R}^d$  according to a probability measure with a *smooth* density  $f_0(x, v)M_\beta(v)$

$$\int_{\mathbb{T}^d \times \mathbb{R}^d} f_0(x, v) M_\beta(v) dx dv = 1.$$

To take into account the exclusion constraint between the hard spheres, we consider ini-

tial distributions of the form

$$f_N(0, Z_N) = \frac{1}{\mathcal{Z}_N^{f_0}} \left( \prod_{i=1}^N f_0(z_i) \right) M_{N,\beta}(Z_N), \quad (2.43)$$

where  $\mathcal{Z}_N^{f_0}$  is the normalization of the probability measure. At low density, Proposition 2.4 ensures that the marginals of the Gibbs measures are very close to a product measure. In the Boltzmann-Grad limit, the density  $\rho$  vanishes as  $\frac{\varepsilon}{\alpha}$  and the proof of Proposition 2.4 can be applied to show that the marginals of the initial data (2.43) factorize asymptotically.

**Proposition 2.7.** *Given  $\beta > 0$ , there is a constant  $C > 0$  (depending linearly on  $\|f_0\|_\infty$ ) such that in the Boltzmann-Grad limit, the following bound holds uniformly in  $s \leq N$  for the marginals  $f_N^{(s)}(0)$  of the initial data*

$$\left| \left( f_N^{(s)}(0) - f_0^{\otimes s} M_\beta^{\otimes s} \right) \mathbf{1}_{\mathbb{D}_\varepsilon^s} \right| \leq C^s \alpha \varepsilon M_\beta^{\otimes s}, \quad (2.44)$$

with the notation

$$f_0^{\otimes s}(Z_s) = \prod_{i=1}^s f_0(z_i).$$

This result shows that the molecular assumption (2.42) holds for the initial data (2.43) in the limit  $\varepsilon \rightarrow 0$ .

**Remark 2.8.** *We stress the fact that the upper bound in (2.44) is relevant only for  $s \ll \log N$  and globally the particles remain correlated even in the Boltzmann-Grad limit. Indeed, the exclusion constraint amounts to conditioning the Lebesgue measure on  $\mathbb{T}^{dN}$  by a set whose probability is given by*

$$\int_{\mathbb{T}^{dN}} \prod_{1 \leq i \neq j \leq N} \mathbf{1}_{|x_i - x_j| > \varepsilon} dX_N = \mathcal{Z}_N,$$

and this probability vanishes in the thermodynamic limit in dimension  $d \geq 3$ . It can be shown that the right hand side of estimate (2.23) captures the correct scaling of  $\mathcal{Z}_N$  in the Boltzmann-Grad limit, i.e.

$$\mathcal{Z}_N \simeq \exp(-N\alpha\varepsilon) \simeq \exp\left(-\alpha \frac{d}{d-1} N \frac{d-2}{d-1}\right),$$

where we used that  $\varepsilon^{1-d} = \frac{N}{\alpha}$ . Thus if  $d \geq 3$ , then  $\mathcal{Z}_N$  tends to 0 which means that in the thermodynamic limit, the Gibbs measure and the Lebesgue measure become singular.

In a breakthrough work [23], Lanford devised an amazing strategy of proof to establish the convergence of the hard-sphere dynamics in the low density limit. The proof has then been improved in a series of works by Cercignani, Illner and Pulvirenti [11], Uchiyama [45], Spohn [40], Gallagher, Saint-Raymond and Texier [15] leading to the following theorem.

**Theorem 2.9.** *Consider a gas of  $N$  hard spheres, initially distributed according to the distribution  $f_N(0)$  introduced in (2.43) where  $f_0 M_\beta$  is a continuous probability density. Then, there exists  $T^* > 0$  (depending only on  $\beta$  and  $\|f_0\|_\infty$ ) such that, in the Boltzmann-Grad limit (2.39), the first marginal  $f_N^{(1)}$  converges on the time interval  $[0, T^*/\alpha]$  to the solution of the Boltzmann equation (2.40).*

The case of particles interacting with a short range potential  $\Phi$  (1.8) was first investigated by King [21] and a complete proof can be found in [15, 30]. Theorem 2.9 will be derived in Chapter 3 as well as a partial form of the molecular chaos (2.42). Note that the convergence is valid only for short times, so that Theorem 2.9 cannot be used to recover the hydrodynamic equations as explained in Section 1.3.

By considering a modified particle dynamics with stochastic collisions, F. Rezakhanlou was able to derive the convergence to the Boltzmann equation for large times [34] as well as the stochastic fluctuations around the limit [33]. We refer to [35] for a review of these results. Boltzmann collision operator has a strong probabilist flavor and several stochastic particle systems have been devised to derive the homogeneous Boltzmann equation. We will not comment further on these approaches as they follow a different route from the one presented in these notes, but we refer the reader to [9, 28] for an overview.

## 2.3 The paradox of the irreversibility

In 1872, Boltzmann's ideas were revolutionary as they opened the way to the description of non-equilibrium phenomena by macroscopic equations. This change of paradigm in the atomistic description led ultimately to the kinetic theory which we know nowadays. However, the Boltzmann equation has first been heavily criticized as it seems to violate some basic physical principles. The first objection was that the time reversibility of the microscopic dynamics is broken by the Boltzmann equation which is irreversible. This is related to the famous  $\mathbb{H}$ -theorem which will be commented in Section 2.3.1. A second paradox, raised by Zermelo in 1896, comes from an apparent contradiction with the Poincaré recurrence Theorem. Indeed, the hard-sphere flow, which is Hamiltonian, is such that any microscopic trajectory of the configurations will come back arbitrarily close to its initial data after a recurrence time. This again appears to be incompatible with the irreversibility of the Boltzmann equation which relaxes towards an equilibrium. In Sections 2.3.2 and 2.3.3, we will introduce two simple dynamics which show that these apparent paradoxes can be solved provided that the microscopic system is considered at an appropriate time scale. We refer to the book [10] for a detailed historical account of the controversies triggered by Boltzmann's work.

### 2.3.1 $\mathbb{H}$ -theorem

Boltzmann understood that the entropy, defined as

$$\mathbb{H}(t) = \int_{\mathbb{T}^d \times \mathbb{R}^d} dx dv f(t, x, v) \log f(t, x, v) \quad (2.45)$$

is monotonous along the flow of the Boltzmann equation (see Theorem 2.10 below) and he related this fact to the second law of thermodynamics. The physical consequence of the entropy dissipation is huge as it implies that Boltzmann equation is *irreversible* which is in contrast to the reversibility of the microscopic hard-sphere dynamics. This paradox was raised by Thomson [43] and Loschmidt [27].

The following theorem shows that the entropy decays in time (note that in physics, entropy is defined with the opposite sign and it is therefore increasing).

**Theorem 2.10** (H-Theorem). *The entropy  $t \mapsto \mathbb{H}(t)$  associated with a solution of Boltzmann equation is nonincreasing. The microscopic entropy*

$$\widehat{\mathbb{H}}(t) = \int_{\mathbb{D}_t^N} dZ_N f_N(t, Z_N) \log f(t, Z_N),$$

*associated with the hard-sphere dynamics is constant in time.*

*Proof.*

**Step 1.** *The mesoscopic entropy.*

For any function  $\varphi$  and any  $x$  in  $\mathbb{T}^d$ , we are first going to derive the following preliminary result

$$\begin{aligned} \int Q(f, f)(x, v) \varphi(v) dv &= \frac{1}{4} \int \left( f(x, v') f(x, v'_1) - f(x, v) f(x, v_1) \right) \\ &\quad \times \left( \varphi(v) + \varphi(v_1) - \varphi(v') - \varphi(v'_1) \right) ((v_1 - v) \cdot v)_+ dv dv_1 dv' \end{aligned} \quad (2.46)$$

This a consequence from the identities below

$$\begin{aligned} &\int Q(f, f)(x, v) \varphi(v) dv \\ &= \int \left( f(x, v') f(x, v'_1) - f(x, v) f(x, v_1) \right) \varphi(v) ((v_1 - v) \cdot v)_+ dv dv_1 dv' \\ &= \frac{1}{2} \int \left( f(x, v') f(x, v'_1) - f(x, v) f(x, v_1) \right) \left( \varphi(v) + \varphi(v_1) \right) ((v_1 - v) \cdot v)_+ dv dv_1 dv' \\ &= -\frac{1}{2} \int \left( f(x, v') f(x, v'_1) - f(x, v) f(x, v_1) \right) \left( \varphi(v') + \varphi(v'_1) \right) ((v_1 - v) \cdot v)_+ dv dv_1 dv', \end{aligned}$$

where we used successively the symmetry between the variables  $v, v_1$  and the fact that the mapping  $(v, v_1, v) \mapsto (v', v'_1, v)$  is an involution which preserves Lebesgue measure.

As  $x$  is fixed, (2.46) can be applied to the function  $\varphi(v) = \log f(x, v)$ , so that

$$\begin{aligned} \int Q(f, f) \log f(x, v) dv &= -\frac{1}{4} \int \left( f(x, v') f(x, v'_1) - f(x, v) f(x, v_1) \right) \log \frac{f(x, v') f(x, v'_1)}{f(x, v) f(x, v_1)} \\ &\quad ((v_1 - v) \cdot v)_+ dv dv_1 dv' \leq 0, \end{aligned} \quad (2.47)$$

where the inequality follows from the fact that

$$\forall a, b \in \mathbb{R}^+, \quad (a - b) \log \frac{a}{b} \geq 0.$$

Taking the derivative of the entropy (2.45) along the flow of the Boltzmann equation, we get

$$\begin{aligned} \partial \mathbb{H}(t) &= \int_{\mathbb{T}^d \times \mathbb{R}^d} dx dv \partial_t f(t, x, v) (1 + \log f(t, x, v)) \\ &= \int_{\mathbb{T}^d \times \mathbb{R}^d} dx dv \operatorname{div}(vf \log f) + Q(f, f) \log f(t, x, v) \leq 0, \end{aligned}$$

where the first term in the integral vanishes by integration by part and the second is non positive thanks to (2.47). This completes the first assertion.



**Step 2.** *The microscopic entropy.*

As the flow  $\mathbf{T}$ . of the microscopic dynamics leaves the Lebesgue measure invariant, we get

$$\widehat{\mathbb{H}}(t) = \int_{\mathbb{D}_\varepsilon^N} dZ_N f_N(0, \mathbf{T}_{-t}(Z_N)) \log f(0, \mathbf{T}_{-t}(Z_N)) = \widehat{\mathbb{H}}(0).$$

Thus the microscopic entropy is time independent.  $\square$

The  $\mathbb{H}$ -Theorem shows that there is a discrepancy between the reversible microscopic dynamics with constant entropy and the entropy dissipation in the kinetic equation. As a consequence, the molecular chaos assumption (2.42) cannot be valid for the full distribution on  $N$  particles. Indeed, if the following approximation by a product measure

$$f_N(t, Z_N) \approx \prod_{i=1}^N f(t, x_i, v_i)$$

was correct then both entropies would be comparable

$$\widehat{\mathbb{H}}(t) = \int_{\mathbb{D}_\varepsilon^N} dZ_N f_N(t, Z_N) \log f(t, Z_N) \approx N \int_{\mathbb{T}^d \times \mathbb{R}^d} dx dv f(t, x, v) \log f(t, x, v) = N\mathbb{H}(t).$$

and this would contradict the  $\mathbb{H}$ -Theorem. As a consequence, the molecular chaos assumption should be questioned and a mathematical justification will be given in Section 3.5. A more in-depth physical discussion on the irreversibility and the arrow of time can be found in [25].

Even though the microscopic evolution is deterministic, the mesoscopic description of the system has a strong probabilist flavor. In particular, we will see in Chapter 4 that a tagged particle behaves as a brownian motion after rescaling. To emphasize the analogy with stochastic processes, we recall below the well known counterpart of the  $\mathbb{H}$ -theorem for Markov chains. For Markov chains, the decay of the relative entropy characterizes the relaxation towards the invariant measure.

For simplicity, we consider a Markov chain  $\{X_t\}_{t \geq 0}$  taking values in  $\mathbb{R}$  with semi-group at time  $t$  given by  $\mathbf{P}_t(x, dy) = P_t(x, y)dy$ . Suppose also that there exists an invariant measure  $\pi(x)dx$  so that

$$\forall y \in \mathbb{R}, \quad \int_{\mathbb{R}} dx \pi(x) P_t(x, y) = \pi(y).$$

For any measure  $\mu$  on  $\mathbb{R}$ , the relative entropy of  $\mu$  with respect to  $\pi$  is defined as

$$\mathbb{H}(\mu|\pi) = \int_{\mathbb{R}} \left( \frac{\mu(x)}{\pi(x)} \log \frac{\mu(x)}{\pi(x)} \right) \pi(x) dx.$$

If  $\mu$  is not absolutely continuous with respect to  $\pi$ , the relative entropy is infinite. Note that the entropy defined in (2.45) is the relative entropy of  $f(t, x, v)$  with respect to the measure  $M_\beta(v)dx dv$  (which is invariant for the Boltzmann equation) with an additional energy term  $\frac{\beta}{2} \int v^2 f(t, x, v) dx dv$ . Since the energy is conserved by the Boltzmann equation, the entropy  $\mathbb{H}(t)$  or the relative entropy are both nonincreasing.

The following theorem shows that the relative entropy associated with the distribution of the Markov chain is monotonous in time.

**Theorem 2.11.** *For any initial probability  $\mu$  and any time  $t \geq 0$ , one has*

$$\mathbb{H}(\mu P_t | \pi) \leq \mathbb{H}(\mu | \pi).$$

*Proof.* We set  $\phi(u) = u \log(u)$ , then

$$\begin{aligned} \mathbb{H}(\mu P_t | \pi) &= \int_{\mathbb{R}} \phi \left( \frac{1}{\pi(x)} \int_{\mathbb{R}} dy \mu(y) P_t(y, x) \right) \pi(x) dx \\ &= \int_{\mathbb{R}} \phi \left( \int_{\mathbb{R}} dy \frac{\mu(y)}{\pi(y)} \frac{\pi(y) P_t(y, x)}{\pi(x)} \right) \pi(x) dx. \end{aligned}$$

Since  $\pi$  is an invariant measure, one can check that  $y \mapsto \frac{\pi(y) P_t(y, x)}{\pi(x)}$  is a probability density on  $\mathbb{R}$

$$\int_{\mathbb{R}} dy \frac{\pi(y) P_t(y, x)}{\pi(x)} = \frac{1}{\pi(x)} \int_{\mathbb{R}} dy \pi(y) P_t(y, x) = \frac{\pi(x)}{\pi(x)} = 1.$$

Thus by Jensen inequality, one has

$$\mathbb{H}(\mu P | \pi) \leq \int_{\mathbb{R}} dx \pi(x) \int_{\mathbb{R}} dy \frac{\pi(y) P_t(y, x)}{\pi(x)} \phi \left( \frac{\mu(y)}{\pi(y)} \right) = \int_{\mathbb{R}} dy \int_{\mathbb{R}} dx \pi(y) P_t(y, x) \phi \left( \frac{\mu(y)}{\pi(y)} \right).$$

Using that  $\int_{\mathbb{R}} dx P_t(y, x) = 1$ , we conclude Theorem 2.11

$$\mathbb{H}(\mu P_t | \pi) \leq \mathbb{H}(\mu | \pi).$$

□

### 2.3.2 Kac ring model

This section is devoted to a simple example of deterministic dynamics exhibiting both a relaxation towards an equilibrium and a recurrence property. This model was devised by Mark Kac in [20] and a very complete review of the model as well as of its physical implications can be found in the article [17].

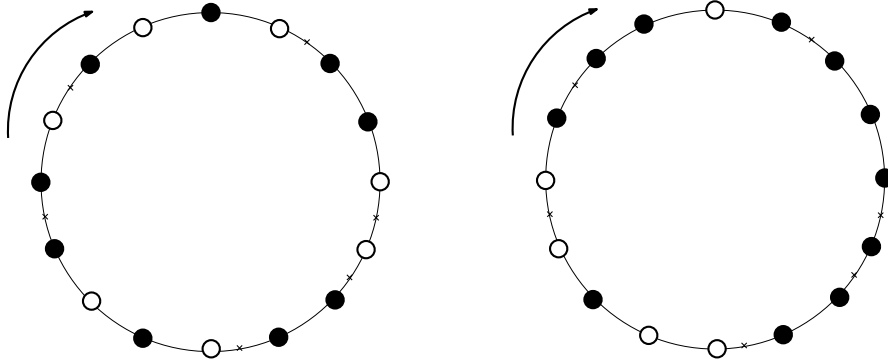


Figure 2.7: Each picture represents a ring with  $N = 16$  colored sites and  $n = 6$  markers depicted by crosses on some edges. The right configuration is deduced from the left configuration after 1 step of the dynamics.

We consider a system of  $N$  sites on a ring and on each site, there is a black or a white ball. Independently on each edge, a marker is placed with probability  $p < 1$  or not with probability  $1 - p$ . The markers are fixed once for all and the initial configuration has  $N$  black balls. At each time step, the balls move clockwise to their neighboring sites. If during a move, a ball crosses an edge with a marker, then this ball changes color (see Figure 2.7).

These dynamical rules are deterministic and reversible: by applying the same rules, but rotating counterclockwise the evolution is reversed. Moreover the system is recurrent because after  $2N$  steps, each ball will be in its initial position and it will have encountered an even number of markers so that its color will be the same as at time 0. In fact, if the number of markers is even initially, then after only  $N$  steps, the initial data is recovered. This second property plays an analogous role to the Poincaré recurrence theorem.

To model the system, it is easier to encode the color of the ball at site  $i$  and time  $t$  by  $\eta_i(t) \in \{-1, 1\}$ . The presence of a marker on the edge  $(i, i + 1)$  is represented by  $m_i = -1$  and its absence by  $m_i = 1$ . The markers are initially placed randomly so that

$$\mathbb{P}(m_i = -1) = p < \frac{1}{2}, \quad \mathbb{P}(m_i = 1) = 1 - p.$$

Thus the colors change according to the rule

$$\forall i \in \{1, \dots, N\}, \quad \eta_{i+1}(t + 1) = m_i \eta_i(t),$$

on the ring the index  $i = N + 1$  is identified with  $i = 1$ . Initially all the balls have the same color  $\eta_i(0) = 1$  and we are interested in the mean evolution of these colors

$$\forall t \geq 1, \quad \mathcal{C}(t) = \sum_{i=1}^N \eta_i(t) = \sum_{i=1}^N m_{i-1} \eta_{i-1}(t-1) = \sum_{i=1}^N m_{i-1} m_{i-2} \dots m_{i-t} \eta_{i-t}(0),$$

where the indices should be understood modulo  $N$ . Using the periodicity of the domain, we recover that for  $\mathcal{C}(2N) = \mathcal{C}(0)$ .

Recall that initially  $\eta_i(0) = 1$  for all site  $i$ . Averaging over the markers and using the fact that all the edges play a symmetric role, we get

$$\mathbb{E}(\mathcal{C}(t)) = N \mathbb{E}(m_1 m_2 \dots m_t).$$

For  $t < N$ , all the markers are independent and the expectation can be computed

$$\mathbb{E}(\mathcal{C}(t)) = N \mathbb{E}(m_1)^t = N(1 - 2p)^t.$$

Since  $t < N$ , the expectation decays exponentially fast and the memory of the initial condition is lost. However correlations start building up for  $t \geq N$  and  $\mathbb{E}(\mathcal{C}(0)) = N$ . Thus this deterministic dynamics exhibits both a fast decay to some disordered state and a recurrence property on larger time scales. This example shows that there is no contradiction to describe an Hamiltonian evolution (as the hard-sphere dynamics) by an irreversible equation (as the Boltzmann equation) if the comparison is achieved on an appropriate time scale.

### 2.3.3 Ehrenfest model

This model has been proposed by Paul and Tatiana Ehrenfest in 1907 [14] in order to settle the controversies on the Boltzmann equation. A beautifully account on this model by Mark Kac can be found in the paper [19].

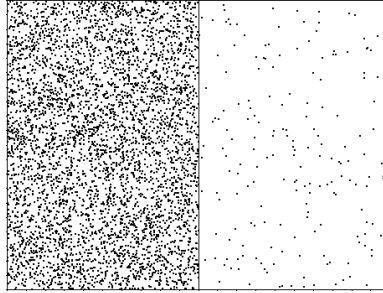


Figure 2.8: At an early stage in the Ehrenfest model, the atoms are mainly on the left side.

Consider a container split into two parts by a wall. The left part of the container is filled by a gas and the right part empty (see Figure 2.8). At time 0, a tiny hole is punctured in the wall so that the gas can reach both sides of the container. The aim of the Ehrenfest model is to describe the relaxation of the gas to its equilibrium state.

To simplify the model, we consider a discrete time and assume that at each time step one atom is chosen randomly among all the atoms and transferred from one side to the other. Let  $X_n$  be the number of atoms in the left compartment at time  $n$  and suppose that initially  $X_0 = K$ . Then  $\{X_n\}_{n \geq 1}$  is a Markov chain taking values in  $\{0, \dots, K\}$  with transition matrix

$$\mathbb{P}(X_{n+1} = \ell - 1 | X_n = \ell) = \frac{\ell}{K}, \quad \mathbb{P}(X_{n+1} = \ell + 1 | X_n = \ell) = \frac{K - \ell}{K}.$$

When the system is at equilibrium, the atoms are uniformly distributed in both sides so that the invariant measure of this Markov chain is

$$\forall \ell \in \{0, \dots, K\}, \quad \pi(\ell) = \frac{1}{2^K} \binom{K}{\ell}.$$

One can easily check that the Markov chain is reversible with respect to  $\pi$

$$\pi(\ell)P(\ell, \ell + 1) = \pi(\ell + 1)P(\ell + 1, \ell).$$

This relation can be interpreted as the stochastic counterpart of the reversibility of the hard-sphere dynamics. Furthermore the Markov chain is irreducible which means that it will visit any configuration in  $\{0, \dots, K\}$  an infinite number of times. If initially the left compartment contains all the particles, then the atoms will first diffuse in the whole container, but then after a very long time, they will eventually all return to the left side. This behavior is analogous to the one predicted by the Poincaré recurrence theorem for Hamiltonian systems.

Thus this simple stochastic model captures two important features of the gas dynamics which are not part of Boltzmann's theory. Fortunately, Ehrenfest model is much simpler to handle than a hard-sphere gas and exact computations can be achieved in order

to quantify the phenomena at play. If the system starts initially with  $X_0 = \ell$ , then the expectation of  $T_\ell$ , the first return time of the Markov chain, at  $\ell$  is given by

$$\mathbb{E}_\ell(T_\ell) = \frac{1}{\pi(\ell)} = 2^K \frac{\ell!(K-\ell)!}{K!}$$

where the subscript in the expectation  $\mathbb{E}_\ell$  stands for the initial state  $X_0 = \ell$ .

When  $K$  is large, say of the order  $10^{23}$ , then

$$\mathbb{E}_K(T_K) = 2^K \quad \text{et} \quad \mathbb{E}_{K/2}(T_{K/2}) \simeq \sqrt{2\pi K}.$$

As a consequence, the first return time to  $K/2$  (which is the mean at equilibrium) will be infinitely shorter than the return time to  $K$ . This latter time is so large that it will never be observed in practice.

The Boltzmann equation describes the typical behavior of a gas and therefore it is conjectured to be valid only on much shorter time scales than the ones involved in the Poincaré recurrence Theorem. Thus the Ehrenfest model solves the apparent contradiction of the paradox raised by Zermelo.



## Chapter 3

# Convergence to the Boltzmann equation

### 3.1 Introduction

The goal of this chapter is to prove the convergence, stated in Theorem 2.9, of the hard-sphere dynamics towards the Boltzmann equation. The following result is a more complete version of Theorem 2.9.

**Theorem 3.1.** *Consider a gas of  $N$  hard spheres, initially distributed according to the distribution*

$$f_N(0, Z_N) = \frac{1}{Z_N^{f_0}} \left( \prod_{i=1}^N f_0(z_i) \right) M_{N,\beta}(Z_N),$$

introduced in (2.43) where the function  $f_0$  satisfies

$$\int_{\mathbb{T}^d \times \mathbb{R}^d} dx dv f_0(x, v) M_\beta(v) = 1, \quad \|f_0\|_{\mathbb{L}^\infty} \leq \exp(-\mu) \quad \text{and} \quad \|\nabla_x f_0\|_{\mathbb{L}^\infty} \leq C, \quad (3.1)$$

for some  $\mu$  in  $\mathbb{R}$  and  $C > 0$ .

There exists  $T^* > 0$  (depending only on  $\beta$ ,  $\mu$  and on the dimension  $d$ ) such that the Boltzmann equation (first introduced in (2.40))

$$\partial_t g + v \cdot \nabla_x g = \alpha Q(g, g) \quad \text{with initial data} \quad g(0, z) = f_0(z) M_\beta(v) \quad (3.2)$$

has a unique solution on the time interval  $[0, T^*/\alpha]$  and the first marginal of the particle system converges to this solution in the Boltzmann-Grad limit  $N\epsilon^{d-1} = \alpha$  (2.39)

$$\forall t \in \left[ 0, \frac{T^*}{\alpha} \right], z \in \mathbb{T}^d \times \mathbb{R}^d, \quad \lim_{N \rightarrow \infty} f_N^{(1)}(t, z) = g(t, z). \quad (3.3)$$

Furthermore, the propagation of chaos holds for any time  $t$  in  $[0, T^*/\alpha]$  and for almost all configurations  $Z_s$  in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$

$$\lim_{N \rightarrow \infty} f_N^{(s)}(t, Z_s) = \prod_{i=1}^s g(t, z_i). \quad (3.4)$$

We stress the fact that the convergence holds only up to a short time of order  $1/\alpha$  (depending on the initial data).

## 3.2 The series expansion

### 3.2.1 Duhamel representation

The marginals are the relevant quantities to describe the gas and they evolve according to the BBGKY hierarchy introduced in Section 2.1.4. Recall that, the evolution of the marginal  $f_N^{(s)}$  of order  $s$  is related, formally, to the marginal  $f_N^{(s+1)}$  of higher order by the following equation

$$\partial_t f_N^{(s)} + \sum_{i=1}^s v_i \cdot \nabla_{x_i} f_N^{(s)} = \alpha C_{s,s+1} f_N^{(s+1)}, \quad (3.5)$$

with specular reflection on the boundary  $\partial\mathbb{D}_\varepsilon^s$  and the collision operator  $C_{s,s+1}$  is given by

$$\begin{aligned} (C_{s,s+1} f_N^{(s+1)})(Z_s) &:= \frac{(N-s)\varepsilon^{d-1}}{\alpha} \\ &\times \left( \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_N^{(s+1)}(\dots, x_i, v'_i, \dots, x_i + \varepsilon v, v'_{s+1}) ((v_{s+1} - v_i) \cdot v)_+ dv dv_{s+1} \right. \\ &\quad \left. - \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_N^{(s+1)}(\dots, x_i, v_i, \dots, x_i + \varepsilon v, v_{s+1}) ((v_{s+1} - v_i) \cdot v)_- dv dv_{s+1} \right). \end{aligned} \quad (3.6)$$

Compared to the definition (2.30) of  $C_{s,s+1}$ , an additional factor  $\alpha$  has been added to match the Boltzmann-Grad scaling.

The solution of a linear PDE with a source term can be represented by using Duhamel's principle which we recall next, in the case of a transport equation in  $\mathbb{D}_\varepsilon^s$  with a source term  $U$

$$\left( \partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i} \right) g(t, Z_s) = U(t, Z_s) \quad \text{with} \quad g(t=0) = g_0. \quad (3.7)$$

The solution of the homogenous part of this equation

$$\left( \partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i} \right) g^1(t, Z_s) = 0 \quad \text{with} \quad g^1(t=0) = g_0,$$

is given in terms of the group  $\mathbf{S}_s$  associated with the transport in  $\mathbb{D}_\varepsilon^s$  which was introduced in (2.31)

$$g^1(t, Z_s) = (\mathbf{S}_s(t)g_0)(Z_s) = g_0(\mathbf{T}_{-t}(Z_s)). \quad (3.8)$$

The part of the equation containing the source term is reduced to

$$\left( \partial_t + \sum_{i=1}^s v_i \cdot \nabla_{x_i} \right) g^2(t, Z_s) = U(t, Z_s) \quad \text{with} \quad g^2(t=0) = 0,$$

and the solution is given by

$$g^2(t, Z_s) = \int_0^t dt_1 (\mathbf{S}_s(t-t_1)U(t_1))(Z_s).$$

Thus the solution of (3.7) is obtained by adding the expressions for  $g^1$  and  $g^2$

$$g(t, Z_s) = (\mathbf{S}_s(t)g_0)(Z_s) + \int_0^t dt_1 (\mathbf{S}_s(t-t_1)U(t_1))(Z_s).$$



The solution of (3.5) can be rewritten by using Duhamel representation

$$f_N^{(s)}(t) = \mathbf{S}_s(t)f_N^{(s)}(0) + \int_0^t dt_1 \mathbf{S}_s(t-t_1)C_{s,s+1}f_N^{(s+1)}(t_1). \quad (3.9)$$

Note that this representation remains as formal as equation (3.5). Indeed the operator  $C_{s,s+1}$  is defined by integrating on sets of codimension 1 and  $f_N^{(s+1)}$  is not regular enough to be well defined on such sets. Besides this technical aspect, the main difficulty is that (3.9) relates the marginal  $f_N^{(s)}$  at time  $t$  to the marginal  $f_N^{(s+1)}$  at an intermediate time in  $[0, t]$ . Since  $f_N^{(s+1)}$  is also unknown, the formula does not seem very helpful. The key idea is to iterate Duhamel formula up to time 0, in order to relate the solution of the BBGKY hierarchy to the initial data

$$f_N^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s(t-t_1)C_{s,s+1}\mathbf{S}_{s+1}(t_1-t_2)C_{s+1,s+2} \dots \mathbf{S}_{s+n}(t_n)f_N^{(s+n)}(0) dt_n \dots dt_1, \quad (3.10)$$

where the term  $n = 0$  stands for the transport part  $\mathbf{S}_s(t)f_N^{(s)}(0)$  without any collision. The order of the marginals in the sum is always less or equal to  $N$  so that the sum is finite. The only source of randomness comes from the initial data and formula (3.10) will allow us to transfert this initial information at positive times. In Section 3.3.2, we will derive uniform estimates in  $N$  in order to control the convergence of this sum.

As in Proposition 2.5, the integration on time in (3.10) provides the missing dimension needed to apply the collision operator  $C_{s,s+1}$ . The iterated Duhamel expansion is derived in the following proposition.

**Proposition 3.2.** *The marginals of the hard-sphere dynamics are given by*

$$\forall s \leq N, \quad f_N^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n Q_{s,s+n}(t)f_N^{(s+n)}(0), \quad (3.11)$$

where the operators are defined as  $Q_{s,s}(t) = \mathbf{S}_s(t)$  and for  $n \geq 1$

$$Q_{s,s+n}(t) := \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s(t-t_1)C_{s,s+1}\mathbf{S}_{s+1}(t_1-t_2)C_{s+1,s+2} \dots \mathbf{S}_{s+n}(t_n)dt_n \dots dt_1. \quad (3.12)$$

*Proof.* By construction,  $f_N(0)$  is bounded from above so that the density  $f_N$  is also bounded by  $\|f_N(0)\|_\infty$  at any time (see Proposition 2.2 on the maximum principle). For the moment, we assume that  $f_N(0)$  is supported in  $\mathcal{D}_\varepsilon^{N,R}$  for some  $R$ . Thus we can use the short time result (2.32) obtained in Proposition 2.5 which is recalled below

$$f_N^{(s)}(t) = \mathbf{S}_s(\delta)f_N^{(s)}(t-\delta) + \alpha \int_{t-\delta}^t dt_1 \mathbf{S}_s(t-t_1)C_{s,s+1}\mathbf{S}_{s+1}(t_1-(t-\delta))f_N^{(s+1)}(t-\delta) + O(\delta^2). \quad (3.13)$$

Compared to (2.32), the factor  $\alpha$  comes from the new normalization (3.6) of the collision operator. As in the derivation of the existence result for the dynamics in Proposition 2.1,

we are going to iterate (3.13) and finally, let  $\delta$  tend to 0. We stress the fact that the error term  $O(\delta^2)$  depends on  $N, \varepsilon, R, \|f_N(0)\|_\infty$ .

Using twice (3.13), we get

$$\begin{aligned}
f_N^{(s)}(t) &= \mathbf{S}_s(2\delta)f_N^{(s)}(t-2\delta) \\
&+ \int_{t-2\delta}^{t-\delta} dt_1 \mathbf{S}_s(\delta) \mathbf{S}_s(t-\delta-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-(t-2\delta)) f_N^{(s+1)}(t-2\delta) \\
&+ \int_{t-\delta}^t dt_1 \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-(t-\delta)) \mathbf{S}_s(\delta) f_N^{(s+1)}(t-2\delta) \\
&+ \int_{t-\delta}^t dt_1 \int_{t-2\delta}^{t-\delta} dt_2 \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-(t-\delta)) \\
&\quad \mathbf{S}_s((t-\delta)-t_2) C_{s+1,s+2} \mathbf{S}_{s+1}(t_2-(t-2\delta)) f_N^{(s+1)}(t-2\delta) + O(3\delta^2) \\
&= \mathbf{S}_s(2\delta) f_N^{(s)}(t-2\delta) \\
&+ \int_{t-2\delta}^t dt_1 \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-(t-2\delta)) f_N^{(s+1)}(t-2\delta) \\
&+ \int_{t-\delta}^t dt_1 \int_{t-2\delta}^{t-\delta} dt_2 \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2} \mathbf{S}_{s+1}(t_2-t-2\delta) f_N^{(s+1)}(t-2\delta) \\
&+ O(3\delta^2).
\end{aligned}$$

The factor 3 has been added in front of the error term to indicate that each iteration induces new error terms of the same type. Indeed (3.13) contains two terms involving  $f_N^{(s)}(t-\delta)$  which lead to two additional contributions of order  $O(\delta^2)$ .

The time interval  $[0, t]$  is split into  $K := t/\delta$  intervals of length  $\delta$  and (3.13) is iterated up to time 0. The order of the marginals has to remain less or equal to  $N$  so that there cannot be more than  $N-s$  collisions. Once the marginal of order  $N$  is reached, it evolves up to time 0 by following the backward hard-sphere flow of the full microscopic dynamics. Note that after  $k$  iterations,  $f_N^{(s)}(t)$  is decomposed into a sum of at most  $N-s$  terms representing the number of collisions up to time  $t-k\delta$ . Thus the next iteration will produce an error of order at most  $NO(\delta^2)$ . Finally, we get

$$\forall s \leq N, \quad f_N^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n Q_{s,s+n}^\delta(t) f_N^{(s+n)}(0) + O(KN\delta^2), \quad (3.14)$$

where the operators are defined as  $Q_{s,s}^\delta(t) = \mathbf{S}_s(t)$  and for  $n \geq 1$

$$Q_{s,s+n}^\delta(t) := \int_{\mathcal{T}_n^\delta} dT_n \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2} \dots \mathbf{S}_{s+n}(t_n), \quad (3.15)$$

and the time integral is over the ordered collision times  $T_n = (t_1, \dots, t_n)$  taking values in the set

$$\mathcal{T}_n^\delta := \left\{ T_n = (t_1, \dots, t_n); \quad t_i \in [t - (k_i - 1)\delta, t - k_i\delta] \right. \\
\left. \text{for a sequence of integers } 0 < k_1 < k_2 < \dots < k_n \leq K \right\}.$$

As in the proof of Proposition 2.1, the error term  $O(KN\delta^2)$  vanishes when  $\delta$  tends to 0 as  $K = t/\delta$ . Furthermore, the modified truncated operator  $Q_{s,s+n}^\delta$  converge to the limit  $Q_{s,s+n}$  (3.12).

Thus identity (3.11) holds for any  $R$ , so that the constraint on the initial data  $f_N(0)$  can be relaxed. This completes the proof of Proposition 3.2.  $\square$

### 3.2.2 The limiting hierarchy and the Boltzmann equation

To study the convergence of the Duhamel representation (3.11) in the Boltzmann-Grad limit, we are going to define the limit of the BBGKY hierarchy which is known as the Boltzmann hierarchy.

In the dilute limit  $\varepsilon \rightarrow 0$ , the hard spheres are converging to points, thus the formal limit of the collision operator is given by

$$\begin{aligned} (C_{s,s+1}^0 g^{(s+1)})(Z_s) &:= \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} g^{(s+1)}(\dots, x_i, v'_i, \dots, x_i, v'_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_+ dv dv_{s+1} \\ &\quad - \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} g^{(s+1)}(\dots, x_i, v_i, \dots, x_i, v_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_- dv dv_{s+1}, \end{aligned} \quad (3.16)$$

where the collision between particles  $i$  and  $s+1$  takes place at  $x_{s+1} = x_i$ . Note also that the prefactor  $\frac{(N-s)\varepsilon^{d-1}}{\alpha}$  in the definition (3.6) of  $C_{s,s+1}$  has been replaced by 1 in the Boltzmann-Grad limit.

As the number of particles  $N$  tends also to infinity, the limiting hierarchy involves an infinite sequence of functions  $\{g^{(s)}(t, Z_s)\}_{s \geq 1}$ . In the limit, the exclusion rule no longer applies so that the function  $g^{(s)}(t)$  takes values in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$  and satisfy the *Boltzmann hierarchy*

$$\partial_t g^{(s)} + \sum_{i=1}^s v_i \cdot \nabla_{x_i} g^{(s)} = \alpha C_{s,s+1}^0 g^{(s+1)}, \quad (3.17)$$

with initial data

$$g^{(s)}(0, Z_s) = \prod_{i=1}^s f_0(z_i) M_\beta^{\otimes s}(V_s). \quad (3.18)$$

Note that the functions  $\{g^{(s)}(t, Z_s)\}_{s \geq 1}$  depend on the parameter  $\alpha$  which controls the frequency of the collision operator in (3.17). As  $\alpha$  is fixed throughout this section, we will omit this dependence in the notation.

In view of Proposition 2.7, the Boltzmann hierarchy is the natural limit for the marginals  $f_N^{(s)}(0)$  at time 0. The solutions of (3.17) will be restricted to continuous function  $g^{(s)}$  in  $\mathbb{T}^{sd} \times \mathbb{R}^{sd}$  which is possible since the free transport preserves continuity on  $\mathbb{T}^{sd} \times \mathbb{R}^{sd}$ . The analog of the operator  $Q_{s,s+n}$  defined in (3.12) is given by

$$Q_{s,s+n}^0(t) := \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s^0(t-t_1) C_{s,s+1}^0 \mathbf{S}_{s+1}^0(t_1-t_2) C_{s+1,s+2}^0 \dots \mathbf{S}_{s+n}^0(t_n) dt_1 \dots dt_n, \quad (3.19)$$

where  $\mathbf{S}_k^0$  is the group associated with the free flow of  $k$  particles on  $\mathbb{T}^{dk} \times \mathbb{R}^{dk}$ . Then the iterated Duhamel formula for the Boltzmann hierarchy takes the form

$$\forall s \geq 1, \quad g^{(s)}(t) = \sum_{n \geq 0} \alpha^n Q_{s,s+n}^0(t) g^{(s+n)}(0). \quad (3.20)$$

The solution of the Boltzmann hierarchy can be explicitly related to the Boltzmann equation.

**Lemma 3.3.** *Let  $g(t, z)$  be a continuous solution of the Boltzmann equation (3.2) with initial data  $g(0, z) = f_0(z)M_\beta(v)$ . Then a solution of the Boltzmann hierarchy (3.17) is given by*

$$\forall s \geq 1, \quad g^{(s)}(t, Z_s) = \prod_{i=1}^s g(t, z_i). \quad (3.21)$$

We stress the fact that the product structure of the initial data (3.18) is kept at positive times in (3.21). Uniqueness of the solution will be derived in Proposition 3.7.

*Proof.* By construction the initial data (3.18) coincide with (3.21) at time 0 and (3.21) satisfies the equations (3.17) for all  $s \geq 1$ .  $\square$

### 3.3 Uniform bounds on the Duhamel series

#### 3.3.1 The Cauchy-Kovalevsky argument

There is still no general theory to ensure existence and uniqueness of solutions of the Boltzmann equation (3.2)

$$\partial_t g + v \cdot \nabla_x g = \alpha Q(g, g)$$

starting from a general initial data  $g(0, z) = f_0(z)M_\beta(v)$ . The main difficulty is that the collision operator  $Q(\cdot, \cdot)$  involves products of the density which would be naturally controlled by  $\mathbb{L}^2$  estimates. Thus the a priori bound on the entropy obtained in IH-Theorem 2.10 is not sufficient to provide a control in time of the  $\mathbb{L}^2$  norm. Nevertheless, the Cauchy problem can be solved globally for small perturbations around an equilibrium density and a notion of weak solutions has been developed by Di Perna and Lions to show the global existence starting from general initial conditions. Further references on the analytical aspects related to the Boltzmann equation can be found in [11].

Solving the Cauchy problem globally in time requires to understand the cancellations between the gain and loss parts of the collision operator. The derivation of the convergence stated in Theorem 3.1 relies on cruder controls which will ensure the existence and uniqueness only for finite time. Indeed, the collision operators in the hierarchies will be estimated by using operators of the form

$$|Q|(f, f)(x, v) := \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} \left( f(x, v') f(x, v'_1) + f(x, v) f(x, v_1) \right) ((v_1 - v) \cdot v)_+ dv_1 dv, \quad (3.22)$$

which do not take into account the cancellations. This procedure will be applied to both hierarchies in Sections 3.3.2 and 3.3.3, but we first discuss some consequences of this approach.

Neglecting the cancellations in the collision operator implies that the solutions cannot be controlled beyond a finite time. Indeed this boils down to considering the following Riccati equation

$$\dot{x}(t) = x(t)^2 \quad \text{with} \quad x(0) = x_0 > 0, \quad (3.23)$$

which blows up in finite time

$$t < \frac{1}{x_0}, \quad x(t) = \frac{x_0}{1 - tx_0}.$$

Following [16] and [11] (page 104), we are going to explain how equation (3.23) is related to the Boltzmann hierarchy and use this correspondence to discuss the uniqueness of the solutions of the hierarchy. Let us start by considering the following hierarchy of ODE

$$\forall k \geq 1, \quad \dot{y}_k(t) = k y_{k+1}(t) \quad \text{with initial data} \quad y_k(0) = y_k^0. \quad (3.24)$$

This hierarchy is related to (3.23) by noticing that

$$\partial_t x(t)^k = k x(t)^{k-1} \dot{x}(t) = k x(t)^{k+1}.$$

One should view the Riccati equation as the analogous of the Boltzmann equation (associated with the operator (3.22)) and the hierarchy (3.24) as a counterpart of the Boltzmann hierarchy introduced in (3.17). This toy model will serve as a benchmark to understand the conditions required for the uniqueness of the solutions of the Boltzmann hierarchy.

First of all, let us check that the uniqueness of the solutions of the hierarchy (3.24) cannot be determined only from the initial data. Indeed, the sequence of constant functions  $y_k(t) = 0$  for all  $k$  is a solution of the hierarchy (3.24) and we are going to construct another solution with the same initial data. Consider the function

$$y_1(t) = \begin{cases} \exp(-\frac{1}{t}), & \text{for } t \geq 0, \\ 0, & \text{for } t \leq 0, \end{cases}$$

which belongs to  $C^\infty(\mathbb{R})$  as all its derivatives at 0 satisfy  $y_1^{(k)}(0) = 0$ . Define recursively a solution of the hierarchy by

$$\forall k \geq 1, \quad y_{k+1}(t) = \frac{1}{k} \dot{y}_k(t) \quad \text{with initial data} \quad y_{k+1}(0) = 0. \quad (3.25)$$

This sequence is also a solution of (3.24) with initial data  $y_k^0 = 0$  for all  $k$ , but it is not real-analytic. Thus additional conditions on the growth of the solutions are required to recover the uniqueness.

We are going to look for solutions  $\{y_k(t)\}_{k \geq 1}$  of (3.24) in the time interval  $[0, T]$  satisfying the growth condition

$$\sup_{t \in [0, T]} \sup_{k \geq 1} |y_k(t)|^{1/k} < \infty. \quad (3.26)$$

In the spirit of Cauchy-Kovalevsky theory, we consider the series associated with a solution of (3.24)

$$U(t, z) = \sum_{k=1}^{\infty} y_k(t) z^{k-1},$$

which are well defined for  $z$  in a neighborhood of 0 under the growth condition (3.26). Differentiating in  $t$ , we get that

$$\partial_t U(t, z) = \sum_{k=1}^{\infty} \dot{y}_k(t) z^{k-1} = \sum_{k=1}^{\infty} k y_{k+1}(t) z^{k-1} = \partial_z U(t, z).$$

Thus the sequence of functions  $\{y_k(t)\}_{k \geq 1}$  is a solution of (3.24) if and only if  $U$  solves the partial differential equation

$$\partial_t U(t, z) = \partial_z U(t, z). \quad (3.27)$$

Given an initial data such that

$$\sup_{k \geq 1} |y_k^0|^{1/k} = \frac{1}{R} < \infty,$$

an explicit solution of (3.27) can be built as follows. Define

$$\forall |z| < R, \quad U^0(z) = \sum_{k=1}^{\infty} y_k^0 z^{k-1},$$

then the unique solution real analytic on the domain  $\{(t, z) \in \mathbb{R}^2, |z| + |r| < R\}$  is given by  $U(t, z) = U^0(t + z)$ . The solution of (3.24) can then be obtained as the Taylor coefficients of the series. The solution of the Riccati equation (3.23) can also be recovered in this way. The growth condition (3.26) is essential to ensure the uniqueness of the solution.

### 3.3.2 Estimates on the BBGKY hierarchy

This section is devoted to the derivation of uniform estimates on the collision operators of the BBGKY hierarchy. We first start by defining an appropriate functional setting.

Proposition 2.7 implies that the marginals of the initial data are uniformly controlled by product measures

$$\forall k \leq N, \quad \left| \left( f_N^{(k)}(0) - f_0^{\otimes k} M_\beta^{\otimes k} \right) \mathbf{1}_{\mathbb{D}_\varepsilon^k} \right| \leq C^k \alpha \varepsilon M_\beta^{\otimes k}.$$

We are going to require that a (weaker) uniform bound holds also at positive times (at least for short times)

$$\forall k \leq N, \quad f_N^{(k)}(t, Z_k) \leq \exp(\gamma k) M_\lambda^{\otimes k}(V_k) \quad \text{for almost all } Z_k \text{ in } \mathbb{D}_\varepsilon^k, \quad (3.28)$$

where  $\lambda$  and  $\gamma$  are parameters to be determined. This growth condition is reminiscent of the condition (3.26) and it provides a control on the velocities (thanks to the parameter  $\lambda$ ) as well as on the local density of the particles (thanks to the parameter  $\gamma$ ). We are going to show that uniform bounds of the type (3.28) are enough to estimate the collision operators.

We start by introducing a functional setting with weighted norms compatible with (3.28). For  $\lambda > 0$  and  $k \geq 1$ , let  $\mathbb{X}_{\varepsilon,k,\lambda}$  be the space of measurable functions  $f_k$  defined almost everywhere on  $\mathbb{D}_\varepsilon^k$  such that

$$\|f_k\|_{\varepsilon,k,\lambda} := \left\| f_k \exp(\lambda H_k) \right\|_{\mathbb{L}^\infty(\mathbb{D}_\varepsilon^k)} < \infty, \quad (3.29)$$

where the Hamiltonian  $H_k(Z_k) = H_k(V_k) = \frac{1}{2} \sum_{i=1}^k |v_i|^2$  was introduced in (2.8).

Neglecting the cancellations between the gain and the loss part of the collision operators as in (3.22), we denote by  $|Q|_{s,s+n}$  the operator obtained by summing the absolute values of all elementary contributions

$$|Q|_{s,s+n}(t) = \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} \mathbf{S}_s(t-t_1) |C_{s,s+1}| \mathbf{S}_{s+1}(t_1-t_2) |C_{s+1,s+2}| \cdots \mathbf{S}_{s+n}(t_n) dt_n \cdots dt_1 \quad (3.30)$$

where the operator  $|C_{s,s+1}|$  is defined for any regular function  $f_{s+1}$  in  $\mathbb{D}_\varepsilon^{s+1}$

$$\begin{aligned} & (|C_{s,s+1}|f_{s+1})(Z_s) \quad (3.31) \\ & := \frac{(N-s)\varepsilon^{d-1}}{\alpha} \left( \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_{s+1}(\dots, x_i, v'_i, \dots, x_i + \varepsilon v, v'_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_+ dv dv_{s+1} \right. \\ & \quad \left. + \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_{s+1}(\dots, x_i, v_i, \dots, x_i + \varepsilon v, v_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_- dv dv_{s+1} \right). \end{aligned}$$

The proposition below provides controls on the norms of the collision operators.

**Proposition 3.4.** *There is a constant  $C$  depending only on the dimension  $d$  such that for all  $s, n \geq 1$  and all  $t \geq 0$ , the operators  $|Q|_{s,s+n}(t)$  satisfy the following continuity estimates. For all  $f_{s+n}$  in  $\mathbb{X}_{\varepsilon,s+n,\lambda}$  then  $|Q|_{s,s+n}(t)f_{s+n}$  belongs to  $\mathbb{X}_{\varepsilon,s,\frac{\lambda}{2}}$  and*

$$\left\| |Q|_{s,s+n}(t)f_{s+n} \right\|_{\varepsilon,s,\frac{\lambda}{2}} \leq \exp(s) \left( \frac{Ct}{\lambda \frac{d+1}{2}} \right)^n \|f_{s+n}\|_{\varepsilon,s+n,\lambda}. \quad (3.32)$$

Note that these estimates involve a loss in the parameter  $\lambda > 0$  and that they deteriorate with time.

*Proof.* We start by estimating the norm of a single collision operator. Let  $f_{k+1}$  be a function in  $\mathbb{X}_{\varepsilon,k+1,\lambda}$ , we are going to prove that for almost all time  $\tau$  and  $k \leq s+n$

$$\left\| |C_{k,k+1}| \mathbf{S}_{k+1}(\tau) f_{k+1} \right\|_{\varepsilon,k+1,(1-\frac{1}{2n})\lambda} \leq \frac{C}{\lambda \frac{d+1}{2}} (s+n) \|f_{k+1}\|_{\varepsilon,k+1,\lambda}. \quad (3.33)$$

The loss in the norm weight has been chosen of order  $\frac{\lambda}{2n}$  in order to iterate  $n$  times this estimate.

The collision operator  $|C_{k,k+1}|$  defined in (3.31) is made of two parts which will be evaluated separately. Since  $N\varepsilon^{d-1} = \alpha$ , the part  $|C_{k,k+1}^+|$  with the scattering is bounded

from above by

$$\begin{aligned}
& (|C_{k,k+1}^+| \mathbf{S}_{k+1}(\tau) f_{k+1})(Z_k) \\
& := \frac{(N-k)\varepsilon^{d-1}}{\alpha} \sum_{i=1}^k \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} dv dv_{k+1} \left( (v_{k+1} - v_i) \cdot v \right)_+ \mathbf{S}_{k+1}(\tau) f_{k+1}(Z'_{k+1}) \\
& \leq \|f_{k+1}\|_{\varepsilon,k+1,\lambda} \sum_{i=1}^k \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} dv dv_{k+1} \left( (v_{k+1} - v_i) \cdot v \right)_+ \mathbf{S}_{k+1}(\tau) \exp(-\lambda H_{k+1}(V'_{k+1})),
\end{aligned}$$

where  $Z'_{k+1}$  stands for the pre-collisional configuration  $(x_1, v_1, \dots, x_i, v'_i, \dots, x_i + \varepsilon v, v'_{k+1})$  and  $V'_{k+1}$  for the corresponding velocities.

Using successively, the conservation of the kinetic energy by scattering  $H_{k+1}(V'_{k+1}) = H_{k+1}(V_{k+1})$  and by the hard-sphere flow, we get the following upper bounds

$$\begin{aligned}
& (|C_{k,k+1}^+| \mathbf{S}_{k+1}(\tau) f_{k+1})(Z_k) \\
& \leq \|f_{k+1}\|_{\varepsilon,k+1,\lambda} \sum_{i=1}^k \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} dv dv_{k+1} \left( (v_{k+1} - v_i) \cdot v \right)_+ \exp(-\lambda H_{k+1}(V_{k+1})) \\
& \leq C \|f_{k+1}\|_{\varepsilon,k+1,\lambda} \int_{\mathbb{R}^d} dv_{k+1} \left( k|v_{k+1}| + \sum_{i=1}^k |v_i| \right) \exp(-\lambda H_{k+1}(V_{k+1})) \\
& \leq C \lambda^{-\frac{d}{2}} \left( k\lambda^{-\frac{1}{2}} + \sum_{i=1}^k |v_i| \right) \exp(-\lambda H_k(Z_k)) \|f_{k+1}\|_{\varepsilon,k+1,\lambda}, \tag{3.34}
\end{aligned}$$

where the last term is obtained by integrating the velocity  $v_{k+1}$ . This upper bound holds for almost all time  $\tau$  and the configuration  $Z_k$ .

As the velocities  $\sum_{i=1}^k |v_i|$  are not bounded, the norm in  $\mathbb{X}_{\varepsilon,k,\lambda}$  of the operator above is infinite. However, by loosing a factor  $\frac{\lambda}{2n}$  on the exponential weight, the sum over the velocities in (3.34) can be controlled thanks to Cauchy-Schwarz estimate

$$\begin{aligned}
& \sum_{i=1}^k |v_i| \exp\left(-\frac{\lambda}{4n} \sum_{1 \leq j \leq k} |v_j|^2\right) \\
& \leq \left(k \frac{2n}{\lambda}\right)^{\frac{1}{2}} \left(\sum_{i=1}^k \frac{\lambda}{2n} |v_i|^2 \exp\left(-\frac{\lambda}{2n} \sum_{j=1}^k |v_j|^2\right)\right)^{1/2} \leq \sqrt{\frac{2nk}{e\lambda}} \leq \sqrt{\frac{2}{e\lambda}}(s+n),
\end{aligned}$$

where we used that  $\|x \exp(-x)\|_\infty \leq e^{-1}$  and that  $k \leq s+n$  in the last inequality. Plugging this inequality in (3.34), we deduce the upper bound (3.33).

The operator  $|Q|_{s,s+n}(t)$  can be estimated by applying iteratively the upper bound (3.33) on the  $n$  collision operators. Each collision operator induces a loss  $\frac{\lambda}{2n}$  on the exponential weight, thus the final estimate is with respect to the norm  $\|\cdot\|_{\varepsilon,k+1,\frac{\lambda}{2}}$ . This leads to an upper of the form  $\frac{C^n}{\lambda^{\frac{(d+1)n}{2}}}(s+n)^n$  uniformly over the collision times  $t_1 > \dots > t_n$ . Integrating then over the times provides an additional factor

$$\int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} dt_n \dots dt_1 = \frac{t^n}{n!}.$$



Finally, we deduce that

$$\left\| |Q|_{s,s+n}(t) f_{s+n} \right\|_{\varepsilon, s, \frac{\lambda}{2}} \leq \frac{(s+n)^n}{n!} \left( \frac{Ct}{\lambda^{\frac{d+1}{2}}} \right)^n \|f_{s+n}\|_{\varepsilon, s+n, \lambda}.$$

Stirling's formula implies that

$$\frac{(s+n)^n}{n!} \leq \exp\left(n \log \frac{n+s}{n} + n\right) \leq \exp(s+n).$$

This completes the upper bound (3.32) on the operator  $|Q|_{s,s+n}(t)$ .  $\square$

The marginals of the BBGKY hierarchy are represented by the iterated Duhamel formula (3.11) in terms on the initial data

$$\forall s \leq N, \quad f_N^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n Q_{s,s+n}(t) f_N^{(s+n)}(0).$$

For sufficiently small times, Proposition 3.4 leads to uniform controls in  $N$  of each term in this sum.

**Proposition 3.5.** *There exists  $T^* > 0$  and a constant  $C > 0$  such that the following upper bound holds uniformly in  $N$  and  $t \in [0, \frac{T^*}{\alpha}]$*

$$\left\| \alpha^n Q_{s,s+n}(t) f_N^{(s+n)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} \leq \left\| \alpha^n |Q|_{s,s+n}(t) f_N^{(s+n)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} \leq \frac{C^s}{2^n}, \quad (3.35)$$

for any  $s \geq 1$  and  $n \geq 0$  such that  $s+n \leq N$ . Both constants  $T^*, C$  depend on  $\|f_0\|_\infty$  and  $\beta$ .

*Proof.* Recall that the marginals of the initial data are uniformly controlled in Proposition 2.7. In particular, the following bound holds for any  $s \geq 1$

$$\forall Z_s \in \mathbb{D}_{\varepsilon'}^s, \quad f_N^{(s)}(0, Z_s) \leq c^s \prod_{i=1}^s f_0(z_i) M_\beta(v_i),$$

for some  $c \geq 1$ . By Assumption (3.1), the function  $f_0$  is bounded from above so that

$$\left\| f_N^{(s)}(0) \right\|_{\varepsilon, s, \beta} \leq C_1^s \exp(-s\mu),$$

for some constant  $C_1$ . Combined with Estimate (3.32) of Proposition 3.4, this implies that

$$\left\| \alpha^n |Q|_{s,s+n}(t) f_N^{(s+n)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} \leq \alpha^n \exp(s) \left( \frac{Ct}{\beta^{\frac{d+1}{2}}} \right)^n C_1^{s+n} \exp(-(s+n)\mu).$$

Thus (3.35) holds for  $t \in [0, \frac{T^*}{\alpha}]$  with

$$T^* = \frac{\beta^{\frac{d+1}{2}}}{C C_1} \exp(\mu). \quad (3.36)$$

$\square$

### 3.3.3 Estimates on the Boltzmann hierarchy

We introduce now the counterpart of the norm (3.29) for the Boltzmann hierarchy. Let  $\mathbb{X}_{0,k,\lambda}$  be the space of continuous functions  $g_k$  defined on  $\mathbb{T}^{dk} \times \mathbb{R}^{dk}$  such that

$$\|g_k\|_{0,k,\lambda} := \sup_{Z_k \in \mathbb{T}^{dk} \times \mathbb{R}^{dk}} |g_k(Z_k) \exp(\lambda H_k(Z_k))| < \infty.$$

The absolute value of the collision operator is denoted by

$$|Q^0|_{s,s+n}(t) = \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s^0(t-t_1) |C_{s,s+1}^0| \mathbf{S}_{s+1}^0(t_1-t_2) |C_{s+1,s+2}^0| \dots \mathbf{S}_{s+n}^0(t_n) dt_n \dots dt_1$$

with

$$\begin{aligned} (|C_{s,s+1}^0| g_{s+1})(Z_s) &:= \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} g_{s+1}(\dots, x_i, v'_i, \dots, x_i, v'_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_+ dv dv_{s+1} \\ &+ \sum_{i=1}^s \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} g_{s+1}(\dots, x_i, v_i, \dots, x_i, v_{s+1}) \left( (v_{s+1} - v_i) \cdot v \right)_- dv dv_{s+1}. \end{aligned}$$

The structure of the operators  $|Q|_{s,s+n}(t)$  and  $|Q^0|_{s,s+n}(t)$  is similar so that the continuity estimates of Proposition 3.4 and 3.5 hold also for the Boltzmann hierarchy.

**Proposition 3.6.** *There is a constant  $C$  depending only on the dimension  $d$  such that for all  $s, n \geq 1$  and all  $t \geq 0$ , the operators  $|Q^0|_{s,s+n}(t)$  satisfy the following continuity estimates. For all  $g_{s+n}$  in  $\mathbb{X}_{0,s+n,\lambda}$ , then  $|Q^0|_{s,s+n}(t)g_{s+n}$  belongs to  $\mathbb{X}_{0,s,\frac{\lambda}{2}}$  and*

$$\left\| |Q^0|_{s,s+n}(t)g_{s+n} \right\|_{0,s,\frac{\lambda}{2}} \leq \exp(s) \left( \frac{Ct}{\lambda^{\frac{d+1}{2}}} \right)^n \|g_{s+n}\|_{0,s+n,\lambda}. \quad (3.37)$$

Furthermore, there exists  $T^* > 0$  and a constant  $C > 0$  such that uniformly in  $s \geq 1, n \geq 0$  and  $t \in [0, \frac{T^*}{\alpha}]$ , one has

$$\left\| \alpha^n Q_{s,s+n}^0(t) g_{\alpha}^{(s+n)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} \leq \left\| \alpha^n |Q^0|_{s,s+n}(t) g_{\alpha}^{(s+n)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} \leq \frac{C^s}{2^n}. \quad (3.38)$$

To investigate the uniqueness of the solutions of the Boltzmann hierarchy, we are going to introduce an appropriate functional setting which takes into account a growth condition as in (3.26). For  $\gamma \in \mathbb{R}$ , we define a norm on the whole sequence  $G = \{g_k\}_{k \geq 1}$  of continuous functions  $g_k$  in  $\mathbb{X}_{0,k,\lambda}$

$$\|G\|_{0,\lambda,\gamma} := \sup_{k \geq 1} \left( \|g_k\|_{0,k,\lambda} \exp(k\gamma) \right)$$

and denote by  $\hat{\mathbb{X}}_{0,\lambda,\gamma}$  the Banach space of functions such that  $\|G\|_{0,\lambda,\gamma} < \infty$ . Given  $T > 0$  and two functions  $\lambda$  and  $\gamma$  in  $[0, T]$ , we also define  $\hat{\mathbb{X}}_{0,\lambda,\gamma,T}$  the space of time continuous functions

$$G : t \in [0, T] \mapsto G(t) = \{g_k(t)\}_{k \geq 1} \in \hat{\mathbb{X}}_{0,\lambda(t),\gamma(t)}$$

endowed with the norm

$$\|G\|_{0,\lambda,\gamma,T} = \sup_{t \in [0,T]} \|G(t)\|_{0,\lambda(t),\gamma(t)}. \quad (3.39)$$

Existence and uniqueness of a solution of the Boltzmann hierarchy follows from the proposition below.

**Proposition 3.7.** *Consider the Boltzmann hierarchy (3.17) starting from the initial data  $G(0) = \{g^{(s)}(0)\}_{s \geq 1}$  in  $\tilde{\mathbb{X}}_{0,\lambda_0,\gamma_0}$  with  $\lambda_0 > 0$ . Then there exists a time  $T^* > 0$  and two decreasing functions  $\lambda > 0$  and  $\gamma$  in the time interval  $[0, \frac{T^*}{\alpha}]$  such that the Boltzmann hierarchy gives rise to a unique solution in  $\tilde{\mathbb{X}}_{0,\lambda,\gamma,\frac{T^*}{\alpha}}$ .*

Note that an explicit solution of the Boltzmann hierarchy was given in (3.21) when the initial data is a product (3.18).

*Proof.* The derivation follows the argument devised in [46] and [15] which is based on Cauchy-Kovalevsky type estimates.

Let  $T^* > 0$  be a parameter to be tuned later and consider the time dependent weights defined in  $[0, \frac{T^*}{\alpha}]$  by

$$\lambda(t) = \lambda_0 - ct \geq \frac{\lambda_0}{2} \quad \text{and} \quad \gamma(t) = \gamma_0 - ct \geq \gamma_0 - \frac{\lambda_0}{2} \quad \text{with} \quad c = \frac{\alpha}{T^*} \frac{\lambda_0}{2}. \quad (3.40)$$

Mild solutions  $G = \{g_k\}_{k \geq 1}$  of the Boltzmann hierarchy are defined for  $t$  in  $[0, \frac{T^*}{\alpha}]$  by

$$G(t) = \mathbf{S}^0(t)g(0) + \alpha \int_0^t dt_1 \mathbf{S}^0(t-t_1) \mathbf{C}^0 G(t_1) dt_1, \quad (3.41)$$

where the transport and the collision operators are acting on each coordinates

$$\forall s \geq 1, \quad (\mathbf{S}^0(t)G)_s = \mathbf{S}_s^0(t)g_s \quad \text{and} \quad (\mathbf{C}^0 G)_s = \mathbf{C}_{s,s+1}^0 g_{s+1}.$$

Proposition 3.7 will follow from a fixed-point theorem. Define the map on  $\tilde{\mathbb{X}}_{0,\lambda,\gamma,\frac{T^*}{\alpha}}$  as

$$\mathcal{F}(G) : t \in \left[0, \frac{T^*}{\alpha}\right] \mapsto \alpha \int_0^t dt_1 \mathbf{S}^0(t-t_1) \mathbf{C}^0 G(t_1) dt_1.$$

We are going to check that for some value of  $T^* > 0$  (which will be determined in (3.43)) then  $\mathcal{F}$  is a contraction in  $\tilde{\mathbb{X}}_{0,\lambda,\gamma,\frac{T^*}{\alpha}}$

$$\|\mathcal{F}(G)\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}} \leq \frac{1}{2} \|G\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}}. \quad (3.42)$$

As a consequence, there exists a unique fixed point in  $\tilde{\mathbb{X}}_{0,\lambda,\gamma,\frac{T^*}{\alpha}}$  which solves (3.41). This completes Proposition 3.7.

We turn now to the proof of (3.42). Fix  $t$  in  $[0, \frac{T^*}{\alpha}]$ . As the free transport preserves the  $\mathbb{L}^\infty$  norm, we get

$$\begin{aligned} & \left\| \int_0^t dt_1 \mathbf{S}_k^0(t-t_1) |C_{k,k+1}^0| g_{k+1}(t_1) \right\|_{0,k,\lambda(t)} \\ & \leq \sup_{Z_k} \int_0^t dt_1 \exp\left(\lambda(t)H_k(Z_k)\right) |C_{k,k+1}^0| |g_{k+1}(t_1)|(Z_k) \\ & \leq \sup_{Z_k} \int_0^t dt_1 \exp\left((\lambda(t) - \lambda(t_1))H_k(Z_k)\right) \frac{C}{\lambda(t_1)^{\frac{d}{2}}} \left(\frac{k}{\lambda(t_1)^{\frac{1}{2}}} + \sum_{i=1}^k |v_i|\right) \|g_{k+1}\|_{0,k+1,\lambda(t_1)}, \end{aligned}$$

where the last inequality is derived as in (3.34).

Using the norm (3.39) defined on the whole sequence  $G(t) = \{g_k(t)\}_{k \geq 1}$ , the following holds for any  $t_1$  in  $[0, \frac{T^*}{\alpha}]$

$$\|g_{k+1}\|_{0,k+1,\lambda(t_1)} \leq \exp(-\gamma(t_1)(k+1)) \|G\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}}.$$

This implies

$$\begin{aligned} & \left\| \int_0^t dt_1 \mathbf{S}_k(t-t_1) |C_{k,k+1}^0| g_{k+1}(t_1) \right\|_{0,k,\lambda(t)} \\ & \leq \|G\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}} \exp(-\gamma(t)(k+1)) \frac{C}{\lambda(t)^{\frac{d}{2}}} \\ & \quad \sup_{Z_k} \int_0^t dt_1 \exp(-c(t-t_1)k) \left(\frac{k}{\lambda(t)^{\frac{1}{2}}} + \sum_{i=1}^k |v_i|\right) \exp(-c(t-t_1)H_k(Z_k)), \end{aligned}$$

where we used that the functions  $\lambda$  and  $\gamma$ , defined in (3.40), are linear and decreasing. Noticing that  $\lambda(t) \geq \frac{\lambda_0}{2}$  and integrating over  $t_1$  leads to the uniform estimate

$$\left\| \int_0^t dt_1 \mathbf{S}_k(t-t_1) |C_{k,k+1}^0| g_{k+1}(t_1) \right\|_{0,\lambda(t),\gamma(t)} \leq \|G\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}} \frac{C \exp(-\gamma(t))}{(\lambda_0/2)^{\frac{d}{2}}} \left(\frac{1}{(\lambda_0/2)^{\frac{1}{2}}} + 1\right) \frac{1}{c}.$$

Replacing  $c$  by its value, we deduce that

$$\|\mathcal{F}(G)\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}} \leq \frac{C \exp(-\gamma_0 - \lambda_0/2)}{(\lambda_0/2)^{\frac{d}{2}} \lambda_0} \left(\frac{1}{(\lambda_0/2)^{\frac{1}{2}}} + 1\right) T^* \|G\|_{0,\lambda,\gamma,\frac{T^*}{\alpha}}.$$

This implies (3.42) when

$$T^* = \frac{(\lambda_0/2)^{\frac{d+3}{2}}}{C(1 + (\lambda_0/2)^{\frac{1}{2}})} \exp(\gamma_0 + \lambda_0/2). \quad (3.43)$$

□

### 3.4 Convergence to the Boltzmann equation

In this section, we are going to derive the first part of Theorem 3.1, i.e. that the typical distribution of a gas particle follows the Boltzmann equation in the Boltzmann-Grad limit. The strategy is to show that the Duhamel series obtained from the BBGKY hierarchy converges to the Duhamel series associated with the Boltzmann hierarchy. The tails of both series can be controlled by the bounds on the collision operators obtained in Section 3.3, but the convergence of the first terms of the series (namely the dominant contribution) requires a more careful analysis. This will be achieved by first interpreting the collision operators in terms of branching processes and then coupling the branching processes associated with both hierarchies.

#### 3.4.1 Collision trees viewed as branching processes

The Duhamel representation (3.11) of the marginal  $f_N^{(1)}$  has an analytic flavor but it can also be interpreted as a branching process of particles evolving according to the hard-sphere dynamics. This is reminiscent of the derivation of Proposition 2.5 where the first order of the Duhamel representation was identified as a collision between two particles.

We will analyze separately each terms in the sum (3.11) of the representation of  $f_N^{(1)}(t)$ . We start with the term of order  $n$

$$Q_{1,n+1}(t)f_N^{(n+1)}(0) = \int_{\mathcal{T}_n} dT_n \mathbf{S}_1(t-t_1)C_{1,2}\mathbf{S}_2(t_1-t_2)C_{2,3}\dots\mathbf{S}_n(t_n)f_N^{(n+1)}(0), \quad (3.44)$$

where the time integral is over the ordered collision times  $T_n = (t_1, \dots, t_n)$  taking values in the set

$$\mathcal{T}_n := \left\{ T_n = (t_1, \dots, t_n); \quad 0 < t_n < \dots < t_2 < t_1 < t \right\}. \quad (3.45)$$

The root of the collision tree is associated with the coordinates  $z_1 = (x_1, v_1) \in \mathbb{T}^d \times \mathbb{R}^d$  of the first particle at time  $t$ . The operator  $\mathbf{S}_1(t-t_1)$  is interpreted as the motion of the first particle following the backward flow up to time  $t_1$  where a collision takes place

$$\forall u \in [t_1, t], \quad z_1(u) = \mathbf{T}_{u-t}(z_1).$$

As in the proof of Proposition 2.5, the collision operator  $C_{1,2}$  is interpreted as the adjunction at time  $t_1$  of a new particle at position  $x_1(t_1) + \varepsilon v_2$  with a deflection angle  $v_2 \in \mathbb{S}^{d-1}$  and with a velocity  $v_2 \in \mathbb{R}^d$ . The new configuration  $Z_2(t_1)$  depends on the type of the collision (see Figure 2.4):

- In the pre-collisional case, i.e. if  $(v_2 - v_1(t_1^+)) \cdot v_2 < 0$ , then the pair of particles is

$$Z_2(t_1) = ((x_1(t_1), v_1), (x_1(t_1) + \varepsilon v_2, v_2)). \quad (3.46)$$

This corresponds to the loss part of the operator  $C_{1,2}$ .

- In the post-collisional case, i.e. if  $(v_2 - v_1(t_1^+)) \cdot v_2 > 0$ , then the pair of particles is defined as the pre-collisional configuration

$$Z_2(t_1) = ((x_1(t_1), v_1'), (x_1(t_1) + \varepsilon v_2, v_2')), \quad (3.47)$$

by using the scattering (2.28). Note that the velocity  $t \mapsto v_1(t)$  is discontinuous at time  $t_1$ . This corresponds to the gain part of the operator  $C_{1,2}$ .

Once created, the new pair of particles evolves according to the backward 2-particle flow during the time interval  $[t_2, t_1]$

$$\forall u \in [t_2, t_1], \quad Z_2(u) = \mathbf{T}_{t_1-u}(Z_2(t_1)).$$

Iterating this procedure, a branching process is built inductively by adding, at time  $t_i$ , a particle labelled  $i + 1$  to the particle with label  $a(i) \leq i$  chosen randomly among the already existing  $i$  particles. Given a deflection angle  $\nu_{i+1}$  and a velocity  $v_{i+1}$ , the velocity of the particle  $a(i)$  and of the new particle  $i + 1$  at time  $t_i$  are updated according to the pre-collisional (3.46) or post-collisional (3.47) rule

$$\begin{cases} Z_{i+1}(t_i) = (\{z_j(t_i)\}_{j \neq a(i)}, (x_{a(i)}(t_i), v_{a(i)}(t_i)), (x_{a(i)}(t_i) + \varepsilon v_{i+1}, v_{i+1})), \\ \quad \text{in the pre-collisional case, i.e. if } (v_{i+1} - v_{a(i)}(t_i)) \cdot \nu_{i+1} < 0, \\ Z_{i+1}(t_i) = (\{z_j(t_i)\}_{j \neq a(i)}, (x_{a(i)}(t_i), v'_{a(i)}(t_i^+)), (x_{a(i)}(t_i) + \varepsilon v_{i+1}, v'_{i+1})), \\ \quad \text{in the post-collisional case, i.e. if } (v_{i+1} - v_{a(i)}(t_i^+)) \cdot \nu_{i+1} > 0. \end{cases}$$

The velocities of the other particles are unchanged. It may happen that the new particle created at position  $x_{a(i)}(t_i) + \varepsilon v_{i+1}$  overlaps with another particle with label in  $\{1, \dots, i\}$ . In this case, the creation is cancelled and the pseudo-trajectory keeps evolving backward with only  $i$  particles. Otherwise, the new configuration follows the backward hard-sphere flow starting from  $Z_{i+1}(t_i)$

$$\forall u \in [t_{i+1}, t_i], \quad Z_{i+1}(u) = \mathbf{T}_{u-t_i}(Z_{i+1}(t_i)).$$

The marginal  $f_N^{(n+1)}(0)$  at time 0 will then be evaluated on the configuration  $Z_{n+1}(0)$  which represents the coordinates of the leaves of the tree.

In between two branching times, the particles in the tree follow the backward hard-sphere flow so that they rebound elastically when they meet. We will call *recollision* these events and the name *collision* will only refer to the creation of a particle at a branching time.

In this way, the operator  $Q_{1,n+1}(t)$  is interpreted in terms of collision trees with  $n$  collisions and the corresponding random process is described by the *pseudo-trajectories* (see Figure 3.1). The pseudo-trajectories are not physical trajectories of the gas particles. They are a geometric interpretation of the iterated Duhamel formula in terms of a branching process flowing backward in time and determined by

- the coordinates  $z_1$  of the initial particle at time  $t$ ,
- the collision times  $T_n = (t_1, \dots, t_n) \in \mathcal{T}_n$  which are interpreted as branching times,
- the labels of the colliding particles  $\mathbf{a} = (a(1), \dots, a(n))$  from which the branchings occur and which take values in the set

$$\mathcal{A}_n := \{\mathbf{a} = (a(1), \dots, a(n)), \quad 1 \leq a(i) \leq i\},$$

- the velocities  $V_{2,n+1} = \{v_2, \dots, v_{n+1}\}$  in  $\mathbb{R}^{dn}$  and deflection angles  $\Theta_{2,n+1} = \{\nu_2, \dots, \nu_{n+1}\}$  in  $S^{(d-1)n}$  for each additional particle.

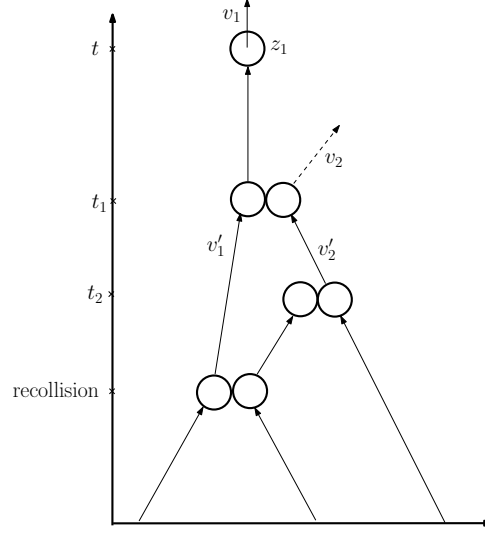


Figure 3.1: A pseudo-trajectory in a collision tree of the BBGKY hierarchy is depicted. The branching process is initialized at time  $t$  with the coordinates  $z_1 = (x_1, v_1)$  of the first particle and then it evolves backwards. At time  $t_1$  the velocity of particle 1 has been changed after the creation of particle 2. Particle 2 has then generated a third particle at time  $t_2$  in a collision without scattering. This third particle recollides with particle 1 and both velocities are modified according to the scattering rule of the hard-sphere dynamics.

For a given collision tree  $\mathbf{a}$  in  $\mathcal{A}_n$ , the variables associated with a pseudo-trajectory will be denoted by

$$\Omega_n = \{T_n, V_{2,n+1}, \Theta_{2,n+1}\} \in \mathcal{T}_n \times \mathbb{R}^{dn} \times \mathbb{S}^{(d-1)n}, \quad (3.48)$$

in order to simplify the notation. We stress the fact that  $\Omega_n$  cannot take any value in  $\mathcal{T}_n \times \mathbb{R}^{dn} \times \mathbb{S}^{(d-1)n}$ : the parameters  $\Omega_n$  leading to an overlap between two particles at a creation time have to be discarded. Indeed, the corresponding pseudo-trajectories are ill-defined.

The contribution (3.44) for  $n$  collisions during  $[0, t]$  can be computed by integrating  $f_N^{(n+1)}(0)$  on the value of the pseudo-trajectories  $Z_{n+1}(0)$  at time 0

$$Q_{1,n+1}(t) f_N^{(n+1)}(0) = \left[ \frac{\varepsilon^{(d-1)n}}{a^n} \prod_{i=1}^n (N-i) \right] \sum_{\mathbf{a} \in \mathcal{A}_n} \int d\Omega_n \mathcal{C}(z_1, \Omega_n) f_N^{(n+1)}(0, Z_{n+1}(0)), \quad (3.49)$$

where the contribution of the cross sections involved in each collision is denoted by

$$\mathcal{C}(z_1, \Omega_n) = \prod_{k=1}^n (v_{k+1} - v_{a(k)}(t_k^+)) \cdot v_{k+1}. \quad (3.50)$$

Note that the contributions of the gain and loss terms in the collision operator  $C_{k,k+1}$  are taken into account by the sign of  $(v_{k+1} - v_{m_k}(t_k^+)) \cdot v_{k+1}$ .

We turn now to the branching process associated with the Boltzmann hierarchy (3.20) and start with the geometric interpretation of the term representing the occurrence of  $n$

collisions

$$Q_{1,n+1}^0(t)g^{(n+1)}(0) = \int_{\mathcal{T}_n} dT_n \mathbf{S}_s^0(t-t_1) C_{1,2}^0 \mathbf{S}_2^0(t_1-t_2) C_{2,3}^0 \cdots \mathbf{S}_{n+1}^0(t_n) g^{(n+1)}(0), \quad (3.51)$$

where we used the previous notation  $T_n = (t_1, \dots, t_n) \in \mathcal{T}_n$ .

The operator  $Q_{1,n+1}^0(t)$  can be represented by collision trees indexed by the coordinates  $z_1^0 = (x_1^0, v_1^0)$  of the first particle at time  $t$ , a collection of branching times  $T_n = (t_1, \dots, t_n)$ , the labels of the colliding particles  $\mathbf{a} = (a(1), \dots, a(n)) \in \mathcal{A}_n$  as well as a collection of velocities  $V_{2,n+1} = \{v_2, \dots, v_{n+1}\}$  in  $\mathbb{R}^{dn}$  and deflection angles  $\Theta_{2,n+1} = \{\nu_2, \dots, \nu_{n+1}\}$  in  $\mathbb{S}^{(d-1)n}$ . If a tree has been built up to time  $t_k$ , then the  $(k+1)$ <sup>th</sup> particle with coordinates  $z_{k+1}^0$  is added at time  $t_k$  at the same position  $x_{a(k)}^0(t_k)$  of the particle  $a(k)$  and their velocities are updated according to the type of the collision:

- if  $(v_{k+1} - v_{a(k)}(t_k)) \cdot v_{k+1} < 0$ , then the new configuration is

$$Z_{k+1}^0(t_i) = (\{z_j^0(t_k)\}_{j \neq a(k)}, (x_{a(k)}^0(t_k), v_{a(k)}(t_k)), (x_{a(k)}^0(t_k), v_{k+1})),$$

- if  $(v_{k+1} - v_{a(k)}(t_k^+)) \cdot v_{k+1} > 0$ , then the new configuration is

$$Z_{k+1}^0(t_i) = (\{z_j(t_k)\}_{j \neq a(k)}, (x_{a(k)}^0(t_k), v'_{a(k)}(t_k^+)), (x_{a(k)}^0(t_k), v'_{k+1})),$$

the velocity of  $a(k)$  is also updated.

During the time interval  $[t_{k+1}, t_k]$ , the corresponding pseudo-trajectory  $Z_{k+1}^0$  evolves according to the backward *free* flow denoted by  $\mathbf{T}_{-u}^0$  until the next particle creation. The collision tree is built backward starting from time  $t$  up to the configuration  $Z_{n+1}^0(0)$  at time 0. We stress the fact that the particles are represented by points which never recollide (almost surely) during the backward evolution. This is a key difference with the pseudo-trajectories in the BBGKY hierarchy. Notice also that when a new particle is created, there is no constraint due to a possible overlap with another particle. Thus the pseudo-trajectories can be parametrized by the variable  $\Omega_n$ , introduced in (3.48), which can take any value in  $\mathcal{T}_n \times \mathbb{R}^{dn} \times \mathbb{S}^{(d-1)n}$ .

The contribution of  $Q_{1,n+1}^0(t)$  can be computed by integrating  $g^{(n+1)}(0)$  on the values of the pseudo-trajectories  $Z_{n+1}^0(0)$  at time 0

$$Q_{1,n+1}^0(t)g^{(n+1)}(0) = \sum_{\mathbf{a} \in \mathcal{A}_n} \int d\Omega_n \mathcal{C}^0(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}^0(0)), \quad (3.52)$$

where the contribution of the cross sections involved in each collision is denoted by

$$\mathcal{C}^0(z_1, \Omega_n) = \prod_{k=1}^n (v_{k+1} - v_{a(k)}(t_k^+)) \cdot v_{k+1}. \quad (3.53)$$

Once again the signs of the gain and loss terms in the collision operator  $C_{k,k+1}^0$  are taken into account by the sign of  $(v_{k+1} - v_{a(k)}(t_k^+)) \cdot v_{k+1}$ . Note that  $\mathcal{C}$  and  $\mathcal{C}^0$  have an identical structure, except that  $\mathcal{C}$  is evaluated on the BBGKY hierarchy pseudo-trajectories and  $\mathcal{C}^0$  on the Boltzmann hierarchy pseudo-trajectories.



### 3.4.2 Coupling the pseudo-trajectories

The collision trees associated with each hierarchy are constructed in a very similar way, and they are encoded by the same set of parameters  $\{z_1, \mathbf{a}, \Omega_n\}$ . However there are two important differences between these trees :

- In the Boltzmann hierarchy, particles are created at the same position of their parent, instead in the BBGKY hierarchy, they are created with a shift of order  $\varepsilon v_i$  which depends on the deflection angle.
- In the Boltzmann hierarchy, particles are points transported by the free flow, thus no recollision occurs. The particles in the pseudo-trajectories of the BBGKY hierarchy bounce elastically when they touch so that the recollisions may modify their trajectories.
- The creation of a particle in the BBGKY hierarchy is discarded if it leads to an overlap with another particle. The overlaps are not a constraint for point particles, so that the occurrence of an overlap induces a discrepancy between the pseudo-trajectories of the two hierarchies.

The discrepancy due to the shifts occurring at each branching times is very small, as the shifts are of order  $\varepsilon$ . A recollision may have much stronger consequences as it can lead to an important modification of the pseudo-trajectory (see Figure 3.2). The overlaps can be treated as local recollisions.

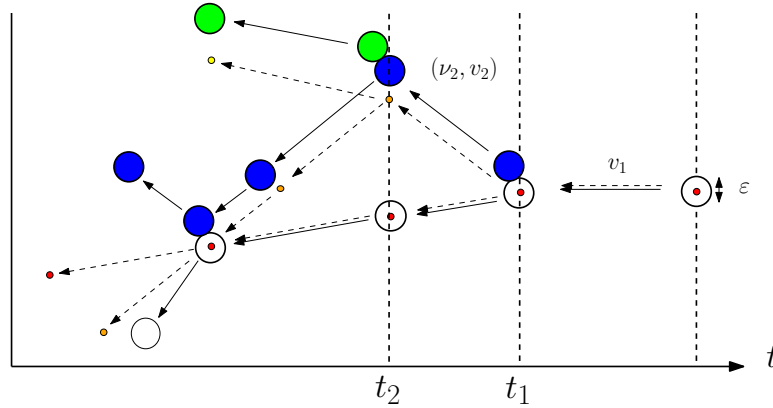


Figure 3.2: The first stages of both pseudo-trajectories are depicted up to the occurrence of a recollision. The BBGKY pseudo-trajectories are represented with plain arrows, whereas the Boltzmann pseudo-trajectories correspond to the dashed arrows. At time  $t$ , the particle with label 1 in the BBGKY hierarchy is a ball of radius  $\varepsilon$  centered at position  $x_1$  and the particle in the Boltzmann hierarchy is depicted as a point located at  $x_1^0 = x_1$ . At time  $t_1$  the second particle is added and at time  $t_2$  the third. Both hierarchies are coupled, but a small error in the particle positions of order  $\varepsilon$  can occur at each collision. In this figure, a recollision between the first and the second particle of the BBGKY pseudo-trajectories occurs and after this recollision the Boltzmann and the BBGKY pseudo-trajectories are no longer close to each other. Indeed the BBGKY trajectories are deflected after the recollision, instead the point particles do not collide and follow a straight line (see the dashed arrows). Note that before the recollision, the trajectories of  $z_1$  and  $z_1^0$  are identical and therefore the plain and the dashed arrows overlap.

In the following proposition, we will show that the iterated Duhamel series of both

hierarchies converge term by term. To do this, it will be enough to check that the recollisions are extremely rare when  $\varepsilon$  tends to 0, so that the two types of pseudo-trajectories can be coupled in order to remain close to each other.

**Proposition 3.8.** *For any time  $t \geq 0$  and any integer  $n$ , the following convergence holds in the Boltzmann-Grad limit*

$$\forall z_1 \in \mathbb{T}^d \times \mathbb{R}^d, \quad \lim_{N \rightarrow \infty} (Q_{1,n+1}(t) f_N^{(n+1)}(0))(z_1) = (Q_{1,n+1}^0(t) g^{(n+1)}(0))(z_1). \quad (3.54)$$

This proposition will be derived by following the approach from [11, 30] and its proof is postponed to Section 3.4.4. Note that a quantitative version of Proposition 3.8 was derived in [15]. We will first use Proposition 3.8 to show the convergence (3.3) of the first marginal towards the solution of the Boltzmann equation.

### 3.4.3 Proof of Theorem 3.1 : convergence to the Boltzmann equation

Recall that from (3.11) and (3.20), the first marginals in the Boltzmann and the BBGKY hierarchies can be rewritten

$$\begin{aligned} f_N^{(1)}(t) &= \sum_{n=0}^{N-1} \alpha^n Q_{s,s+n}(t) f_N^{(s+n)}(0), \\ g^{(1)}(t) &= \sum_{n \geq 0} \alpha^n Q_{s,s+n}^0(t) g^{(s+n)}(0). \end{aligned}$$

Furthermore by Proposition 3.7, the solution of the Boltzmann hierarchy is unique in the time interval  $[0, \frac{T^*}{\alpha}]$  and it coincides with the solution of the Boltzmann equation  $g^{(1)}(t, z_1) = g(t, z_1)$  thanks to Lemma 3.3. Thus it is enough to show that  $f_N^{(1)}(t)$  converges to  $g^{(1)}(t)$  in order to prove that it converges to the solution of the Boltzmann equation.

For any  $\delta > 0$ , one can find an integer  $K$ , thanks to Propositions 3.5 and 3.6, such that for any  $t \in [0, \frac{T^*}{\alpha}]$  and uniformly in  $N > K$

$$\sum_{n=K}^{N-1} \left\| \alpha^n Q_{1,n+1}(t) f_N^{(n+1)}(0) \right\|_{\varepsilon, 1, \frac{\beta}{2}} + \sum_{n=K}^{\infty} \left\| \alpha^n Q_{1,n+1}^0(t) g^{(n+1)}(0) \right\|_{0, 1, \frac{\beta}{2}} \leq \delta. \quad (3.55)$$

Using (3.11) and (3.20), we deduce

$$f_N^{(1)}(t) - g^{(1)}(t) = \sum_{n=0}^K \alpha^n \left( Q_{1,n+1}(t) f_N^{(n+1)}(0) - Q_{1,n+1}^0(t) g^{(n+1)}(0) \right) + O(\delta).$$

Thus the convergence of the first marginal for any  $t \in [0, \frac{T^*}{\alpha}]$  and  $z_1$  in  $\mathbb{T}^d \times \mathbb{R}^d$

$$\lim_{N \rightarrow \infty} f_N^{(1)}(t, z_1) = g^{(1)}(t, z_1)$$

follows from the convergence of the first  $K$  terms proved in Proposition 3.8 (and then by letting  $\delta$  tend to 0). This completes the first part of Theorem 3.1.

### 3.4.4 Proof of Proposition 3.8

We first check that instead of  $Q_{1,n+1}(t)f_N^{(n+1)}(0)$  introduced in (3.49), it is enough to consider

$$\widehat{Q}_{1,n+1}(t)f_N^{(n+1)}(0) = \sum_{\mathbf{a} \in \mathcal{A}_n} \int d\Omega_n \mathcal{C}(z_1, \Omega_n) f_N^{(n+1)}(0, Z_{n+1}(0)), \quad (3.56)$$

as the prefactor

$$\frac{\varepsilon^{(d-1)n}}{\alpha^n} \prod_{i=1}^n (N-i) = \prod_{i=1}^n \left(1 - \frac{i}{N}\right) = 1 + O\left(\frac{n^2}{N}\right), \quad (3.57)$$

is asymptotically close to 1 thanks to the Boltzmann-Grad scaling  $N\varepsilon^{(d-1)} = \alpha$ .

Using the representations (3.52) and (3.56) in terms of the pseudo-trajectories, the difference can be decomposed as

$$\begin{aligned} & \widehat{Q}_{1,n+1}(t)f_N^{(n+1)}(0) - Q_{1,n+1}^0(t)g^{(n+1)}(0) \\ &= \sum_{\mathbf{a} \in \mathcal{A}_n} \left[ \int d\Omega_n \left( \mathcal{C}(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}(0)) - \mathcal{C}^0(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}^0(0)) \right) \right. \\ & \quad \left. + \int d\Omega_n \mathcal{C}(z_1, \Omega_n) \left( f_N^{(n+1)}(0, Z_{n+1}(0)) - g^{(n+1)}(0, Z_{n+1}(0)) \right) \right], \end{aligned} \quad (3.58)$$

where the pseudo-trajectories in each integral are evaluated with the same branching structure given by the collision tree  $\mathbf{a}$ . Note that overlaps may occur in the BBGKY hierarchy, in this case the pseudo-trajectories are discarded and the corresponding terms in the integrals are set equal to 0.

Using the definition (3.18) of  $g^{(n+1)}(0)$ , the last term in (3.58) can be easily estimated by Proposition 2.7 which implies that the initial densities are close

$$\begin{aligned} & \left| \int d\Omega_n \mathcal{C}(z_1, \Omega_n) \left( f_N^{(n+1)}(0, Z_{n+1}(0)) - g^{(n+1)}(0, Z_{n+1}(0)) \right) \right| \\ & \leq C^n \alpha \varepsilon \int d\Omega_n \left| \mathcal{C}(z_1, \Omega_n) \right| M_\beta^{\otimes(n+1)}(Z_{n+1}(0)) \\ & \leq C^n \alpha \varepsilon \left( |Q|_{1,1+n}(t) M_\beta^{\otimes(n+1)} \right)(z_1). \end{aligned}$$

Given  $z_1$  and  $n$ , the last term is linear in  $\varepsilon$ . Thus when  $\varepsilon$  tends to 0, the last term in (3.58) vanishes.

We turn now to the estimation of the difference of the first two terms in (3.58). This is a key point of the proof as it boils down to controlling the recollisions and the overlaps which may occur in the pseudo-trajectories. Indeed, two pseudo-trajectories  $Z_{n+1}, Z_{n+1}^0$  encoded by the same parameters  $\{z_1, \Omega_n\}$  are close if the BBGKY pseudo-trajectory has no recollision and no overlap :

$$\forall i \leq n+1, \forall t \in [0, t_{i-1}], \quad |x_i(t) - x_i^0(t)| \leq (i-1)\varepsilon \quad \text{and} \quad v_i(t) = v_i^0(t), \quad (3.59)$$

with the notation  $t_0 = t$ . When there are no recollisions, the velocities are updated only at the collision times and besides the shift of the positions by  $\varepsilon$  at the creation times, both

pseudo-trajectories evolve exactly in the same way. At the creation time of particle  $i$  the cumulated error of these shifts is at most  $(i-1)\varepsilon$ .

If (3.59) holds, we deduce from the expression (3.18) of the initial data that

$$\begin{aligned} \left| g^{(n+1)}(0, Z_{n+1}(0)) - g^{(n+1)}(0, Z_{n+1}^0(0)) \right| &= M_\beta^{\otimes n+1}(V_{n+1}) \left| \prod_{i=1}^{n+1} f_0(z_i) - \prod_{i=1}^{n+1} f_0(z_i^0) \right| \\ &\leq \|\nabla_x f_0\|_\infty \|f_0\|_\infty^n M_\beta^{\otimes n+1}(V_{n+1})(n+1)^2 \varepsilon, \end{aligned} \quad (3.60)$$

where we used that  $\nabla_x f_0$  is bounded to estimate from above the small shifts of the positions of the pseudo-trajectories. Therefore, for the collision parameters  $\Omega_n$  such that the pseudo-trajectories have no overlap and no recollisions, the right hand side of (3.58) tends to 0. It remains to show that the occurrence of the recollisions and of the overlaps are so rare that they do not contribute to the difference in (3.58).

For a given collision tree  $\mathbf{a}$  and an initial data  $z_1$ , we are going to compare the pseudo-trajectories from both hierarchies associated with the same collection of parameters  $\Omega_n$  introduced in (3.48). In probabilistic terms, both pseudo-trajectories are coupled with the same source of randomness. We define below  $\mathcal{G}_\varepsilon$  a set of *good* parameters for which there will be no recollisions or overlaps

$$\mathcal{G}_\varepsilon = \left\{ \Omega_n = \{T_n, V_{2,n+1}, \Theta_{2,n+1}\}, \right. \quad (3.61)$$

$$\forall i, j \in \{1, \dots, n+1\}, i \not\sim j, \forall u \in [0, t], \quad |x_i^0(u) - x_j^0(u)| \geq 4n\varepsilon,$$

$$\forall i \in \{2, \dots, n+1\}, \forall u \in \left[ 0, t_{i-1} - \frac{4n\varepsilon}{|v_{i+1}(t_{i-1}) - v_{a(i)}(t_{i-1})|} \right], \quad |x_i^0(u) - x_{a(i)}^0(u)| \geq 4n\varepsilon,$$

$$\forall i \in \{1, \dots, n-1\}, \quad t_{i+1} < t_i - \frac{4n\varepsilon}{|v_{i+1}(t_i) - v_{a(i)}(t_i)|} \Big\},$$

where the symbol  $i \not\sim j$  means that  $i$  is different from  $j$  and that  $i$  and  $j$  are not related by a branching (i.e  $i \neq a(j)$  or  $j \neq a(i)$ ). Note that  $\mathcal{G}_\varepsilon$  depends on  $z_1$  which is fixed throughout the proof.

The set  $\mathcal{G}_\varepsilon$  is indexed by the pseudo-trajectories of the Boltzmann hierarchy and the Lebesgue measure of its complement  $\mathcal{G}_\varepsilon^c$  will be shown to converge to 0. We are first going to check that a parameter  $\Omega_n$  in  $\mathcal{G}_\varepsilon$  generates a BBGKY pseudo-trajectory without collision or overlap. The idea is that if the particles in a Boltzmann pseudo-trajectory remain far apart from each other then the corresponding BBGKY pseudo-trajectories cannot have any recollision because both trajectories have to be close thanks to (3.59).

Given  $\Omega_n$  a set of parameters in  $\mathcal{G}_\varepsilon$ , we are going to build the BBGKY and Boltzmann pseudo-trajectories inductively. Suppose that both pseudo-trajectories have evolved during the time interval  $[s, t]$  and that no recollisions or overlaps have occurred so far. We are going to check that the conditions on the parameters in  $\mathcal{G}_\varepsilon$  implies that the next creations will not lead to a recollision or an overlap:

- The first condition in (3.61) implies that particles in a Boltzmann pseudo-trajectory with labels  $i \not\sim j$  are at distance at least  $4n\varepsilon$  thus the corresponding particles in the Boltzmann pseudo-trajectories will remain at distance  $2n\varepsilon$  thanks to (3.59). Notice also that when particles are far enough, then no overlap can occur when a new particle is created.

- When a particle is created, it is close to its parent for some time (depending on their relative velocity), but then both particles depart from each other. However, due to a future collision (which would deflect the trajectory) or due to the periodicity of  $\mathbb{T}^d$ , a particle and its parents might get closer at a later time and the second condition in (3.61) has been added to forbid this eventuality.
- Finally the third condition in (3.61) implies that two particle creations do not occur in a very short amount of time. Indeed when a new particle  $i$  is created, it is very close to its parent  $a(i)$ , thus if a third particle is created, by  $i$  or  $a(i)$ , immediately after then it may lead to an overlap or a recollision between these 3 particles. The third condition implies that particles  $i$  and  $a(i)$  drift at distance  $4n\varepsilon$  before any creation of a new particle.

As the pseudo-trajectories of the BBGKY hierarchy indexed by parameters in  $\mathcal{G}_\varepsilon$  have no recollisions, the difference in (3.58) can be decomposed as

$$\begin{aligned} & \int d\Omega_n \left( \mathcal{C}(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}(0)) - \mathcal{C}^0(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}^0(0)) \right) \\ &= \int d\Omega_n \mathbf{1}_{\{\Omega_n \notin \mathcal{G}_\varepsilon\}} \left( \mathcal{C}(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}(0)) - \mathcal{C}^0(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}^0(0)) \right) \\ &+ \int d\Omega_n \mathbf{1}_{\{\Omega_n \in \mathcal{G}_\varepsilon\}} \mathcal{C}(z_1, \Omega_n) \left( g^{(n+1)}(0, Z_{n+1}(0)) - g^{(n+1)}(0, Z_{n+1}^0(0)) \right), \end{aligned}$$

where we used the fact that for  $\Omega_n \in \mathcal{G}_\varepsilon$ , there is no recollision or overlap and the velocities of both pseudo-trajectories coincide so that  $\mathcal{C}(z_1, \Omega_n) = \mathcal{C}^0(z_1, \Omega_n)$ .

Applying inequality (3.60) to control the trajectory without recollisions, we get

$$\begin{aligned} & \left| \int d\Omega_n \left( \mathcal{C}(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}(0)) - \mathcal{C}^0(z_1, \Omega_n) g^{(n+1)}(0, Z_{n+1}^0(0)) \right) \right| \\ & \leq \|f_0\|_\infty^{n+1} \int d\Omega_n \mathbf{1}_{\{\Omega_n \notin \mathcal{G}_\varepsilon\}} \left( |\mathcal{C}(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}) + |\mathcal{C}^0(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}^0) \right) \\ & + \|\nabla_x f_0\|_\infty \|f_0\|_\infty^n (n+1)^2 \varepsilon \int d\Omega_n \mathbf{1}_{\{\Omega_n \in \mathcal{G}_\varepsilon\}} |\mathcal{C}(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}). \end{aligned} \quad (3.62)$$

When  $\varepsilon$  tends to 0, the sets  $\mathcal{G}_\varepsilon^c$  are going to converge to

$$\begin{aligned} \mathcal{N}_0 = \left\{ \Omega_n = \{T_n, V_{2,n+1}, \Theta_{2,n+1}\}, \right. & \quad (3.63) \\ & \exists i, j \in \{1, \dots, n+1\}, i \neq j, \exists u \in [0, t], \quad |x_i^0(u) - x_j^0(u)| = 0, \\ & \exists i \in \{2, \dots, n+1\}, \exists u < t_{i-1}, \quad |x_i^0(u) - x_{a(i)}^0(u)| = 0, \\ & \left. t_n < t_{n-1} < \dots < t_2 < t_1 \right\}. \end{aligned}$$

For any fixed  $z_1$ ,  $\mathcal{N}_0$  has measure 0. Indeed, suppose that  $x_i^0(u) = x_j^0(u)$  at some time  $u$  and denote by  $u' \in [u, t]$  the time of the last deflection of the particle  $i$  or  $j$ . Then the constraint  $x_i^0(u) = x_j^0(u)$  forces the collision parameters at time  $u'$  to be in a set of measure 0. Thus we deduce that for almost all  $\Omega_n$

$$\lim_{\varepsilon \rightarrow 0} \mathbf{1}_{\mathcal{G}_\varepsilon^c}(\Omega_n) = \mathbf{1}_{\mathcal{N}_0}(\Omega_n) = 0.$$

The dominated convergence theorem implies the following convergence for any  $z_1$

$$\lim_{\varepsilon \rightarrow 0} \int d\Omega_n \mathbf{1}_{\{\Omega_n \notin \mathcal{G}_\varepsilon\}} \left( |\mathcal{C}(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}) + |\mathcal{C}^0(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}^0) \right) = 0, \quad (3.64)$$

where the domination relies on the comparison of the term in parenthesis with the collision operators which are both finite (Propositions 3.4 and 3.6)

$$|Q|_{1,1+n}(t) M_\beta^{\otimes(n+1)}(z_1) < \infty \quad \text{and} \quad |Q^0|_{1,1+n}(t) M_\beta^{\otimes(n+1)}(z_1) < \infty.$$

The last term in (3.62) can be bounded in the same way.

$$\varepsilon \int d\Omega_n \mathbf{1}_{\{\Omega_n \in \mathcal{G}_\varepsilon\}} |\mathcal{C}(z_1, \Omega_n)| M_\beta^{\otimes n+1}(V_{n+1}) \leq \varepsilon |Q|_{1,1+n}(t) M_\beta^{\otimes(n+1)}(z_1).$$

Thus this term also tends to 0 and this concludes the proof of Proposition 3.8.

## 3.5 The molecular chaos assumption

### 3.5.1 Convergence of the marginals

In this section, we complete the derivation of Theorem 3.1 and show that the marginals asymptotically factorize (3.4). Using the explicit solution of the Boltzmann hierarchy derived in Lemma 3.3, this boils down to checking that for any time  $t$  in  $[0, T^*/\alpha]$  and for almost all configurations  $Z_s$  in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$

$$\lim_{N \rightarrow \infty} f_N^{(s)}(t, Z_s) = g^{(s)}(t, Z_s). \quad (3.65)$$

As for the convergence of the first marginal, the proof is based on the comparison of the Duhamel series (3.11) and (3.20)

$$f_N^{(s)}(t) - g^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n Q_{s,s+n}(t) f_N^{(s+n)}(0) - \sum_{n=0}^{\infty} \alpha^n Q_{s,s+n}^0(t) g^{(s+n)}(0).$$

Using Propositions 3.5 and 3.6, one can show as in (3.55) that for any  $\delta > 0$ , there is  $K$  large enough such that for any  $t \in [0, \frac{T^*}{\alpha}]$  and uniformly in  $N \geq s + K$

$$\sum_{n=K}^{N-s} \left\| \alpha^n Q_{s,n+s}(t) f_N^{(n+s)}(0) \right\|_{\varepsilon, s, \frac{\beta}{2}} + \sum_{n=K}^{\infty} \left\| \alpha^n Q_{s,n+s}^0(t) g^{(n+s)}(0) \right\|_{0, s, \frac{\beta}{2}} \leq \delta. \quad (3.66)$$

Thus it is enough to generalize Proposition 3.8 and to show that for any time  $t \geq 0$  and any integer  $n$ , then the following convergence holds for almost all initial data  $Z_s$  in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$

$$\forall t \in \left[ 0, \frac{T^*}{\alpha} \right], \quad \lim_{N \rightarrow \infty} (Q_{s,n+s}(t) f_N^{(n+s)}(0))(Z_s) = (Q_{s,n+s}^0(t) g^{(n+s)}(0))(Z_s). \quad (3.67)$$

The convergence (3.65) can then be deduced by combining (3.66) and (3.67).

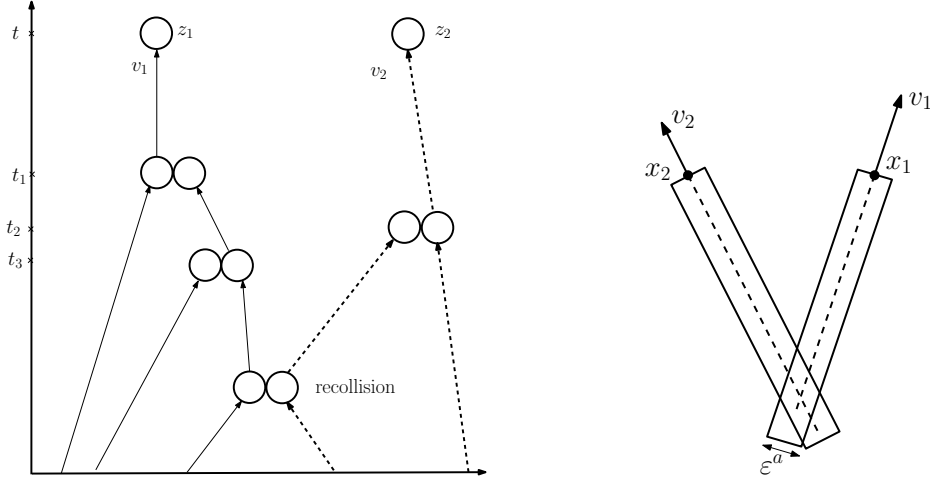


Figure 3.3: Computing the marginal  $f_N^{(2)}(t, z_1, z_2)$  boils down to controlling the pseudo-trajectories with 2 roots at time  $t$  (see the figure on the left). The collision tree associated with the second particle is in dashed lines to distinguish it from the tree associated with the first particle. The correlations between the two particles are related to the recollisions between the two collision trees. The configuration  $(z_1, z_2)$ , depicted on the right, belongs to the set  $\mathcal{B}_0^2$  as the trajectories intersect in the past. The enlarged set of pathological configurations  $\mathcal{B}_\varepsilon^2$  should be understood as the set of configurations such that the tubes of width  $\varepsilon^a$  around the backward trajectories intersect.

The proof of (3.67) follows the same pattern as the argument of Proposition 3.8, nevertheless there is an important twist as the convergence does not hold for all configurations  $Z_s$ . The main steps of the derivation are described below. The operators  $Q_{s,s+n}(t)$  and  $Q_{s,s+n}^0(t)$  can be also represented by collision trees. The main difference is that the pseudo-hierarchies are now encoded by  $s$  trees with roots at time  $t$  indexed by the coordinates of each of the  $s$  particles  $Z_s$  or  $Z_s^0$ . These trees are built inductively by evolving backward in time and new particles are created at each branching time. Once again a major difference between both hierarchies comes from the recollisions. In the Boltzmann hierarchy, the particles evolve according to the free flow and therefore do not interact with each other except possibly at the creation of a new particle. Thus the collision trees associated with the configuration  $Z_s^0$  are the union of the  $s$  non-interacting collision trees starting from the roots  $z_1^0, z_2^0, \dots, z_s^0$  at time  $t$ . For the BBGKY hierarchy the  $s$  trees are no longer independent as the pseudo-trajectories can be modified by the recollisions either between particles belonging to the same collision tree or between particles belonging to collision trees generated at time  $t$  by different roots (see Figure 3.3). To control the recollisions, one has to show that the pseudo-trajectories encoded by the parameters  $\Omega_n$  in the set  $\mathcal{G}_\varepsilon^c$  (3.61) have a vanishing contribution when  $\varepsilon$  tends to 0. We stress the fact that  $\mathcal{G}_\varepsilon^c$  depends on the configuration  $Z_s$  at time  $t$ . Contrary to the case  $s = 1$ , this will have important consequences. Indeed for  $s = 1$ , the limiting set  $\mathcal{N}_0$  introduced in (3.63) has measure 0 for any given configuration  $z_1$ . This is no longer the case for  $s > 1$  if the configuration  $Z_s$  belongs to the set

$$\mathcal{B}_0^s = \left\{ Z_s \in \mathbb{T}^{ds} \times \mathbb{R}^{ds}, \quad \exists i \neq j, \exists u \in [0, t], \quad |(x_i - uv_i) - (x_j - uv_j)| = 0 \right\} \quad (3.68)$$

such that two particles will encounter along the backward free flow starting from  $Z_s$

(see Figure 3.3). Indeed, for any configuration  $Z_s$  in  $\mathcal{B}_0^s$  there is a set of parameters  $\Omega_n$  of positive measure such that the pseudo-trajectories starting from  $Z_s$  will have a recollision for any  $\varepsilon > 0$ . Nevertheless, one can check that, for  $Z_s$  outside  $\mathcal{B}_0^s$ , the limiting set

$$\begin{aligned} \mathcal{N}_0^s = \left\{ \Omega_n = \{T_n, V_{2,n+1}, \Theta_{2,n+1}\}, \right. \\ \left. \begin{aligned} &\exists i, j \in \{1, \dots, n+s\}, i \not\sim j, \exists u \in [0, t], \quad |x_i^0(u) - x_j^0(u)| = 0, \\ &\exists i \in \{s+1, \dots, n+s\}, \exists u < t_{i-s}, \quad |x_i^0(u) - x_{a(i)}^0(u)| = 0, \\ &t_n < t_{n-1} < \dots < t_2 < t_1 \end{aligned} \right\}. \end{aligned}$$

has measure 0 and the dominated convergence theorem can be applied as in (3.64). This completes the convergence (3.67) for any configuration  $Z_s$  outside  $\mathcal{B}_0^s$ . Since  $\mathcal{B}_0^s$  has measure 0 in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$ , the convergence (3.65) of the  $s$  marginal holds for almost all configurations  $Z_s$  in  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$ .

### 3.5.2 Quantitative estimates

The convergence in Theorem 3.1 can be improved in order to quantify the distance between the marginal  $f_N^{(s)}$  and its limit  $g^{(s)}$ . This was first initiated in [15] and developed in [30, 31, 12, 7].

Before stating the convergence result, we introduce the sets which can lead to recollisions in the pseudo-trajectories starting from configurations with  $s$  particles. This boils down to enlarging the set  $\mathcal{B}_0^s$  introduced in (3.68). Given  $a \in (0, 1)$  and  $T^*$ , we set

$$\mathcal{B}_\varepsilon^s = \left\{ Z_s \in \mathbb{T}^{ds} \times \mathbb{R}^{ds}, \quad \exists i \neq j, \exists u \in \left[0, \frac{T^*}{\alpha}\right], \quad |(x_i - uv_i) - (x_j - uv_j)| \leq \varepsilon^a \right\}. \quad (3.69)$$

The following theorem summarizes the results derived in [15, 12, 7]. An extension of this result to soft potentials has been proven in [15, 30].

**Theorem 3.9.** *Under the assumptions of Theorem 3.1 on the initial data, the marginal  $f_N^{(s)}$  converges, in the Boltzmann-Grad limit, to  $g^{(s)}$  uniformly on the configurations  $Z_s$  in  $\mathbb{D}_\varepsilon^s \setminus \mathcal{B}_\varepsilon^s$ , i.e. there exists  $T^* > 0$  such that*

$$\forall t \in \left[0, \frac{T^*}{\alpha}\right], \quad \left| (f_N^{(s)}(t, Z_s) - g^{(s)}(t, Z_s)) \mathbf{1}_{\{Z_s \notin \mathcal{B}_\varepsilon^s\}} \right| \leq C^s M_{\frac{\beta}{2}}^{\otimes s}(V_s) \gamma(\varepsilon),$$

where the function  $\gamma(\varepsilon)$  converges to 0 as  $\varepsilon$  tends to 0. The rate of convergence depends on the parameter  $a$  which controls the set of initial data (3.69).

For any given  $\varepsilon$ , the configurations in the set  $\mathcal{B}_\varepsilon^s$  are excluded as they could potentially lead to recollisions. When  $\varepsilon$  tends to 0, these sets shrink to the set  $\mathcal{B}_0^s$  defined in (3.68) and therefore Theorem 3.9 implies the factorization (3.4).

Let us briefly review the new ideas involved in the proof of Theorem 3.9. In the derivation of Theorem 3.1, all the estimates were explicit in  $\varepsilon$  with the exception of the control on the recollisions in Proposition 3.8 which relied on the dominated convergence



theorem. Thus the key step is to estimate the size of  $\mathcal{N}_\varepsilon$  (3.61) in terms of  $\varepsilon$ . Restricting to configurations  $Z_s$  in the complement of  $\mathcal{B}_\varepsilon^s$  means that the particles remains at distance  $\varepsilon^a \gg \varepsilon$  from each other when they evolve according to backward transport. When a new particle is created, one has to prove that the probability that a recollision occurs with another particle is small. Indeed, a recollision requires to aim, at the creation time, very precisely at a small ball of size  $\varepsilon$  at distance at least  $\varepsilon^a$  and this imposes strong constraints on the collision parameters at the creation time of a particle. By evaluating at each new collision the range of the parameters which would lead to a recollision, upper bounds on the measure of  $\mathcal{N}_\varepsilon$  can be obtained [15, 30].

We will not derive Theorem 3.9, nevertheless the ideas mentioned previously will be key for the study of the large time asymptotics and they will be detailed in Chapters 4 and ??.

The function  $\gamma(\varepsilon)$ , introduced in Theorem 3.9, can be estimated and one can show that  $\gamma(\varepsilon)$  decays to 0 as  $\varepsilon^{a'}$  for some  $a' < 1$ . Thus Theorem 3.9 implies the convergence of all the marginals of order  $s \ll \log N$ . By studying the cumulants instead of the marginals, Pulvirenti and Simonella [31] were able to prove that the correlations of much higher order tend to 0. Let  $\{\varphi_k\}_{k \geq 1}$  be a sequence of smooth functions in  $\mathbb{T}^d \times \mathbb{R}^d$  uniformly bounded and define the empirical averages at time  $t$  of these functions as well as their limits by

$$\forall k \geq 1, \quad F_k(Z_N(t)) = \frac{1}{N} \sum_{i=1}^N \varphi_k(z_i(t)), \quad \widehat{\varphi}_k(t) = \int_{\mathbb{T}^d \times \mathbb{R}^d} dz \varphi_k(z) g_\alpha(t, z),$$

where  $g_\alpha$  is the solution of the Boltzmann equation. The idea is to consider the correlations for some  $p > 0$

$$\sup_{j < \varepsilon^{-p}} \mathbb{E}_N \left( \prod_{k=1}^j (F_k(Z_N(t)) - \widehat{\varphi}_k(t)) \right), \quad (3.70)$$

which take into account many cancelations. In a slightly different setting than the one presented here (i.e. under a grand-canonical initial measure and with the hard-sphere dynamics in  $\mathbb{R}^d$ ) it is proven in [31], that there exists  $p > 0$  and a time  $T^* > 0$  such that (3.70) converges to 0 when  $\varepsilon$  tends to 0.

### 3.5.3 Time reversal and propagation of chaos

The Boltzmann equation was derived heuristically under the molecular chaos assumption stated in (2.42) which requires a very quantitative version of the factorization when two particles are in contact with each other

$$f_N^{(2)}(t, x_1, v_1, x_1 - \varepsilon v, v_2) \approx f_N^{(1)}(t, x_1, v'_1) f_N^{(1)}(t, x_1, v'_2). \quad (3.71)$$

Lanford's strategy does not rely on the molecular chaos assumption and the proof of the convergence does not provide any clue for closing directly the equations of the BBGKY hierarchy : the convergence holds for the whole hierarchy. The factorization of the marginals is only recovered in the limit (3.65) by using the fact that the solution of the

Boltzmann hierarchy is itself factorized

$$\lim_{N \rightarrow \infty} f_N^{(s)}(t, Z_s) = g^{(s)}(t, Z_s) = \prod_{i=1}^s g(t, z_i). \quad (3.72)$$

In fact, this convergence does not hold for all the configurations  $Z_s$ . In particular, the configurations in the set  $\mathcal{B}_0^s$  (3.68) have been excluded as they lead to recollisions. Furthermore, the propagation of chaos (3.72) is valid only for fixed  $Z_s$  in the limit  $N \rightarrow \infty$  and more quantitative bounds on the factorization would be needed to be used in the proof of the convergence towards the Boltzmann equation. For a given  $\varepsilon$ , the convergence could not be proved in Theorem 3.9 for the configurations in the set  $\mathcal{B}_\varepsilon^s$ . This shows that the convergence derived in Theorem 3.9 is very far from establishing the kind of estimate required by the molecular chaos assumption (3.71). In fact, excluding the configurations leading to recollisions is not a technical necessity, but a necessary condition to prove the convergence towards an irreversible equation.

Theorem 3.9 implies the convergence of the marginals on the time interval  $[0, \frac{T^*}{\alpha}]$ . The microscopic hard-sphere dynamics is reversible, thus if all the velocities are flipped at the intermediate time  $\tau = \frac{T^*}{2\alpha}$  then the particle system returns to its initial state. As the Boltzmann equation is not reversible, the reversed equation is the backward Boltzmann equation and Lanford's strategy cannot apply to the microscopic dynamics starting from the density at time  $\tau$  with the reversed velocities, i.e. from the distribution

$$\widehat{f}_N(0, Z_N) = f_N(\tau, \mathcal{R}(Z_N)).$$

The iterated Duhamel formula (3.11) applied to this initial data implies that for  $t \in [0, \tau]$

$$\widehat{f}_N^{(1)}(t) = \sum_{n=0}^{N-1} \alpha^n Q_{1,n+1}(t) \widehat{f}_N^{(n+1)}(0). \quad (3.73)$$

By the reversibility of the microscopic dynamics

$$\widehat{f}_N^{(1)}(t, x, v) = f_N^{(1)}(\tau - t, x, -v).$$

Evaluating the term  $Q_{1,n+1}(t) \widehat{f}_N^{(n+1)}(0)$  in (3.73) amounts to integrate  $\widehat{f}_N^{(n+1)}(0, Z_{n+1})$  over the configurations  $Z_{n+1}$  of the pseudo-trajectories. Reversing the velocities, one has

$$\widehat{f}_N^{(n+1)}(0, Z_{n+1}) = f_N^{(n+1)}(\tau, \mathcal{R}(Z_{n+1})).$$

By construction of the pseudo-trajectories (see Figure 3.4), the configuration  $\mathcal{R}(Z_{n+1})$  arises from a branching process thus it belongs to the set  $\mathcal{B}_\varepsilon^s$  (with  $a = 1$ ) as the particles have to recollide in the backward hard-sphere flow. Therefore, the configurations needed to compute the reverse dynamics are exactly those which were discarded in Theorem 3.9. This means that the molecular chaos assumption cannot hold for the configurations  $Z_s$  in  $\mathcal{B}_\varepsilon^s$  (with  $a = 1$ )

$$f_N^{(s)}(\tau, Z_s) \not\approx g^{(s)}(\tau, Z_s),$$

otherwise the system would converge towards the Boltzmann equation and not the backward Boltzmann equation. The marginal  $f_N^{(s)}(t)$  is almost factorized, but it lacks regularity on very specific sets which have a vanishing measure with  $\varepsilon$ . Once the rare events

leading to recollisions have been neglected, some information on the reversibility has been lost so that the initial state cannot be recovered by running the dynamics backward. Thus the irreversibility of the limiting process comes from this loss of memory. The key role of the recollision and the importance of the sets  $\mathcal{B}_0^s$  defined in (3.68) has been first emphasized in [47] and a more quantitative discussion on the size of the pathological sets  $\mathcal{B}_\varepsilon^s$  can be found in [7].

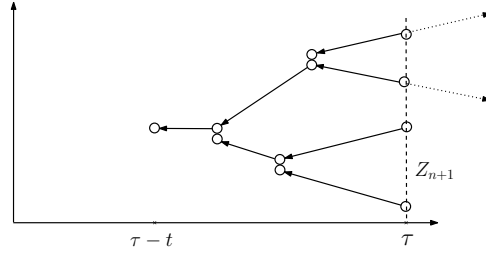


Figure 3.4: At time  $\tau$ , all the velocities are flipped and the system restarts from the density  $\widehat{f}_N(0, Z_N) = f_N(\tau, \mathcal{R}(Z_N))$ . The pseudo-trajectory associated with the reversed evolution  $\widehat{f}_N^{(1)}(t, x, v)$  form a branching process with final configurations  $Z_{n+1}$  in the set  $\mathcal{B}_\varepsilon^s$ .



# Chapter 4

## Tagged particle

### 4.1 Introduction

R. Brown (1828), A. Einstein (1905), J. Perrin (1909)

The main goal of this chapter is to show that a stochastic process can arise from purely deterministic dynamics.

### 4.2 The ideal gas

#### 4.2.1 A Markov chain representation

The simplest model of a tagged particle in an ideal gas is a stochastic process such that the particle moves in a straight line and at random times changes its direction according to random kicks. In this setting, the gas molecules do not interact with each other and they simply act on the tagged particle as a thermal bath at a given temperature  $1/\beta$ .

The tagged particle velocity  $\{v(t)\}_{t \geq 0}$  is then a Markov chain evolving according to the following stochastic rule. If the tagged particle has a velocity  $v$ , it will keep this velocity up to an exponential time  $\mathcal{T}$  with rate  $\alpha a(v)$  defined as

$$\mathbb{P}(\mathcal{T} \geq u) = \exp(-\alpha a(v)) \quad \text{and} \quad a(v) = \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} ((w-v) \cdot \nu)_+ M_\beta(w) dw d\nu,$$

then at time  $\mathcal{T}$ , the velocity is updated to

$$v' = v - ((v-w) \cdot \nu) \nu,$$

where the parameters  $w$  and  $\nu$  are chosen according to the probability density

$$\frac{((w-v) \cdot \nu)_+ M_\beta(w)}{a(v)} dw d\nu.$$

This amounts to say that a particle with velocity  $w$ , chosen randomly according to the Maxwellian distribution  $M_\beta$ , collides with the tagged particle according to a law depending on the relative velocity  $w-v$  and on a random impact parameter  $\nu$ .

This procedure is then iterated to build the random sequence of collisions and the path of the Markov chain  $\{v(t)\}_{t \geq 0}$ . The ideal gas is uniformly distributed therefore the collision mechanism is independent of the position of the tagged particle which evolves simply according to

$$x(t) = \int_0^t ds v(s). \quad (4.1)$$

This stochastic evolution mimics the collisions encountered by a tagged particle in a dilute gas. Nevertheless contrary to the deterministic gas dynamics, the spatial structure is neglected and the Markov chain is memoryless. This means that the trajectory of an incoming particle at velocity  $w$  will not influence the tagged particle beyond the collision. As a consequence, the outgoing velocity  $w'$  plays no role in the evolution of the tagged particle : the momentum and the energy are no longer conserved by the stochastic process which is dissipative.

Rephrasing the previous discussion, we say that the Markov chain  $\{v(t)\}_{t \geq 0}$  has a generator given by  $\alpha \mathcal{L}$  with

$$\mathcal{L}\varphi(v) := \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} (\varphi(v') - \varphi(v)) ((w - v) \cdot v)_+ M_\beta(w) dw dv, \quad (4.2)$$

and  $\mathcal{L}$  is known as the *linear Boltzmann operator*. The proposition below summarizes some properties of  $\mathcal{L}$ .

**Proposition 4.1.** *The operator  $\mathcal{L}$  is self-adjoint in  $\mathbb{L}^2(M_\beta)$ , which amounts to say that the stochastic process  $\{v(t)\}_{t \geq 0}$  is reversible with respect to its invariant measure  $M_\beta$ . Furthermore,  $-\mathcal{L}$  has a spectral gap, i.e. that there exists  $c > 0$  such that for any  $\varphi$  in  $\mathbb{L}^2(M_\beta)$*

$$\mathbb{E}_{M_\beta}(\varphi^2) - \left(\mathbb{E}_{M_\beta}(\varphi)\right)^2 \leq -c \mathbb{E}_{M_\beta}(\varphi \mathcal{L}\varphi), \quad (4.3)$$

for some  $c > 0$ .

*Proof.* Recall that the map  $\mathcal{J} : (v, w, \nu) \mapsto (v', w', -\nu)$  introduced in (2.5) is an involution and preserves the Lebesgue measure. Noticing that

$$M_\beta^{\otimes 2}(v', w') = M_\beta^{\otimes 2}(v, w) \quad \text{and} \quad ((w - v) \cdot \nu)_+ = ((w' - v') \cdot \nu)_-,$$

we get, for any functions  $\psi$  and  $\varphi$  in  $\mathbb{L}^2(M_\beta)$ , that

$$\int_{\mathbb{S}^{d-1} \times \mathbb{R}^{2d}} dv dv' dw M_\beta^{\otimes 2}(v, w) \psi(v) \varphi(v') ((w - v) \cdot \nu)_+ \quad (4.4)$$

$$= \int_{\mathbb{S}^{d-1} \times \mathbb{R}^{2d}} dv dv' dw M_\beta^{\otimes 2}(v', w') \psi(v) \varphi(v') ((w' - v') \cdot \nu)_- \quad (4.5)$$

$$= \int_{\mathbb{S}^{d-1} \times \mathbb{R}^{2d}} dv dv' dw M_\beta^{\otimes 2}(v, w) \psi(v') \varphi(v) ((w - v) \cdot \nu)_+, \quad (4.6)$$

where second equality is obtained by the change of variables  $\mathcal{J}$ . Identity (4.4) implies that  $\mathcal{L}$  is self-adjoint in  $\mathbb{L}^2(M_\beta)$

$$\mathbb{E}_{M_\beta}(\psi \mathcal{L}\varphi) = \int M_\beta^{\otimes 2}(v, w) \psi(v) (\varphi(v') - \varphi(v)) ((w - v) \cdot \nu)_+ = \mathbb{E}_{M_\beta}(\varphi \mathcal{L}\psi).$$

Thus the stochastic process is reversible with respect to the measure  $M_\beta$  and  $M_\beta$  is the invariant measure.

Using the identity (4.4), we get also that  $\mathcal{L}$  has a negative spectrum

$$\mathbb{E}_{M_\beta}(\varphi \mathcal{L}\varphi) = -\frac{1}{2} \int M_\beta^{\otimes 2}(v, w) (\varphi(v') - \varphi(v))^2 ((w - v) \cdot v)_+ \leq 0.$$

We refer to [37] for a proof of the spectral gap.  $\square$

The semigroup of the Markov process is denoted by

$$P_t = \exp(t\alpha\mathcal{L}). \quad (4.7)$$

The number of random kicks per unit of time is of order  $1/\alpha$ . We stress that the prefactor  $\alpha$  plays a role similar to the factor  $\alpha$  in the Boltzmann-Grad scaling  $\alpha = Ne^{d-1}$ . When  $\alpha$  tends to infinity, the collision frequency increases which boils down to saying that the density of the particles in the bath is increasing.

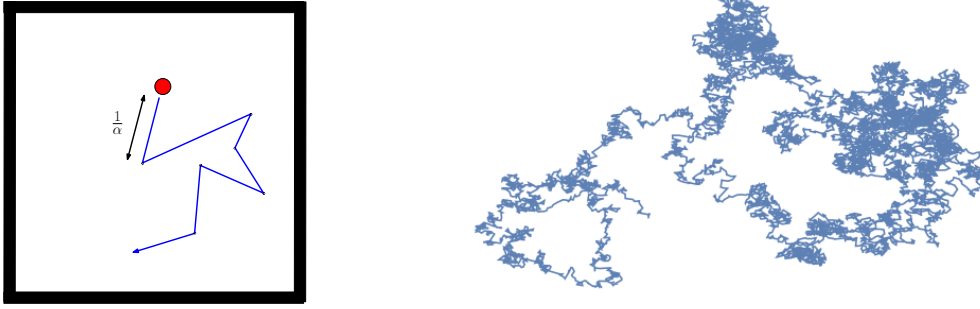


Figure 4.1: The typical time between two collisions in the stochastic process is  $1/\alpha$ . Thus in a time  $t = \alpha\tau$ , the position is the sum of roughly  $\alpha^2\tau$  random displacements of size  $1/\alpha$ . A Brownian path is depicted on the right.

The density  $g_\alpha(t, x, v) = \varphi_\alpha(t, x, v)M_\beta(v)$  of the tagged particle is given in terms of  $\varphi_\alpha$ , the solution of the *linear Boltzmann equation*

$$\partial_t \varphi_\alpha + v \cdot \nabla_x \varphi_\alpha = \alpha \mathcal{L} \varphi_\alpha, \quad (4.8)$$

with initial data  $\varphi_0(x, v)$ . We stress the fact that the structure of the linear Boltzmann equation is reminiscent to the one of the Boltzmann equation. We refer to [9, 28] for a survey on the probabilist representations of the Boltzmann equation.

We are interested in the large time behavior of the position of the tagged particle  $x(t)$  (4.1). After an appropriate space/time rescaling, the process is expected to converge to a Brownian motion. Instead of rescaling space, it will be more convenient to consider the limit  $\alpha \rightarrow \infty$  of the following processes

$$\forall \alpha > 0, \quad \chi_\alpha(\tau) = x(\alpha\tau) \quad (4.9)$$

starting at  $\chi_\alpha(0) = 0$  with initial velocity distributed according to  $M_\beta$ . In this limit,  $\tau$  stands for the macroscopic time and the number of random kicks scales as  $\alpha t = \alpha^2\tau$  and each increment is of order  $\frac{1}{\alpha}$ . Thus this is the correct scaling in  $\alpha$  to observe a central limit theorem and it is not necessary to rescale the position (see Figure 4.1).

**Theorem 4.2.** *The sequence of processes  $\{\chi_\alpha\}_{\alpha>0}$  converges in law to a Brownian motion in  $\mathbb{R}^d$  with diagonal diffusion matrix  $\mathbf{D} \text{Id}$  where the diffusion coefficient is given by*

$$\mathbf{D} = \frac{1}{d} \mathbb{E}_{M_\beta} \left( v \cdot (-\mathcal{L})^{-1} v \right). \quad (4.10)$$

The proof is standard and the main arguments are sketched in Section 4.2.2.

In the rest of this section, we justify the form of the diffusion coefficient  $\mathbf{D}$  and check that it is given in terms of the limiting variance of the process. Given an orthonormal basis  $\{e_1, \dots, e_d\}$ , the coordinates of the process in  $\mathbb{R}^d$  are denoted by

$$\forall i \leq d, \quad x_{e_i}(t) = x(t) \cdot e_i, \quad v_{e_i}(t) = v(t) \cdot e_i.$$

We are going to show that for any  $\tau > 0$

$$\lim_{\alpha \rightarrow \infty} \mathbb{E}_{M_\beta} \left( x_{e_1}(\alpha\tau)^2 \right) = 2\mathbf{D}\tau. \quad (4.11)$$

The other covariances can be computed in the same way.

To prove (4.11), we first use the fact that  $M_\beta$  is the invariant measure in order to rewrite

$$\begin{aligned} \mathbb{E}_{M_\beta} \left( x_{e_1}(\alpha\tau)^2 \right) &= \mathbb{E}_{M_\beta} \left( \int_0^{\alpha\tau} ds \int_0^{\alpha\tau} ds' v_{e_1}(s) v_{e_1}(s') \right) \\ &= 2 \int_0^{\alpha\tau} ds \int_s^{\alpha\tau} ds' \mathbb{E}_{M_\beta} \left( v_{e_1}(0) v_{e_1}(s' - s) \right). \end{aligned}$$

Changing variables and integrating by parts, we deduce that

$$\begin{aligned} \mathbb{E}_{M_\beta} \left( x_{e_1}(\alpha\tau)^2 \right) &= 2 \int_0^{\alpha\tau} ds \int_0^{\alpha\tau-s} du \mathbb{E}_{M_\beta} \left( v_{e_1}(0) v_{e_1}(u) \right) \\ &= 2\alpha\tau \int_0^{\alpha\tau} ds \frac{s}{\alpha\tau} \mathbb{E}_{M_\beta} \left( v_{e_1}(0) v_{e_1}(\alpha\tau - s) \right) \\ &= 2\alpha\tau \int_0^\infty ds \left( 1 - \frac{s}{\alpha\tau} \right)_+ \mathbb{E}_{M_\beta} \left( v_{e_1}(0) v_{e_1}(s) \right). \end{aligned}$$

This can be rephrased in terms of the semigroup  $P_s = \exp(\alpha s \mathcal{L})$

$$\begin{aligned} \mathbb{E}_{M_\beta} \left( x_{e_1}(\alpha\tau)^2 \right) &= 2\alpha\tau \int_0^\infty ds \left( 1 - \frac{s}{\alpha\tau} \right)_+ \mathbb{E}_{M_\beta} \left( v_{e_1} P_s v_{e_1} \right) \\ &= 2\tau \int_0^\infty du \left( 1 - \frac{u}{\alpha^2\tau} \right)_+ \mathbb{E}_{M_\beta} \left( v_{e_1} \exp(u\mathcal{L}) v_{e_1} \right), \end{aligned} \quad (4.12)$$

where the scaling of the generator has been absorbed in the change of variable  $u = \alpha s$ . As the process is reversible, the right hand side of the identity is nonnegative

$$\mathbb{E}_{M_\beta} \left( v_{e_1} \exp(u\mathcal{L}) v_{e_1} \right) = \mathbb{E}_{M_\beta} \left( \left( \exp\left(\frac{u}{2}\mathcal{L}\right) v_{e_1} \right)^2 \right) \geq 0.$$

By the monotone convergence theorem, the limiting variance converges to

$$\mathbb{E}_{M_\beta} \left( x_{e_1}(\alpha\tau)^2 \right) = 2\tau \int_0^\infty du \mathbb{E}_{M_\beta} \left( v_{e_1} \exp(u\mathcal{L}) v_{e_1} \right) = 2\tau \mathbb{E}_{M_\beta} \left( v_{e_1} (-\mathcal{L})^{-1} v_{e_1} \right). \quad (4.13)$$

Recall, from Proposition 4.1, that  $-\mathcal{L}$  has a spectral gap so that the inverse  $(-\mathcal{L})^{-1} v_{e_1}$  is well defined. This completes the proof of (4.11).



### 4.2.2 Proof of Theorem 4.2

Fix  $\mathcal{T} > 0$ . To prove the convergence, in Theorem 4.2, of the processes  $\chi_\alpha$  in the time interval  $[0, \mathcal{T}]$  towards a Brownian motion  $B$  with variance  $\mathbf{D} \text{Id}$ , it is enough (see [5], Chapter 2) to check that

- the convergence of the marginals at different times  $\tau_1 < \tau_2 < \dots < \tau_\ell \leq \mathcal{T}$

$$\lim_{\alpha \rightarrow \infty} \mathbb{E}_{M_\beta} \left( h_1(\chi_\alpha(\tau_1)) \dots h_\ell(\chi_\alpha(\tau_\ell)) \right) = \mathbb{E} \left( h_1(B(\tau_1)) \dots h_\ell(B(\tau_\ell)) \right), \quad (4.14)$$

where  $\{h_1, \dots, h_\ell\}$  is a collection of continuous functions in  $\mathbb{R}^d$ .

- the tightness of the sequence, that is for any  $\tau \in [0, \mathcal{T}]$

$$\forall \delta > 0, \quad \lim_{\eta \rightarrow 0} \lim_{\alpha \rightarrow \infty} \mathbb{P}_{M_\beta} \left( \sup_{\tau < \sigma < \tau + \eta} |\chi_\alpha(\sigma) - \chi_\alpha(\tau)| \geq \delta \right) = 0. \quad (4.15)$$

The main ingredients for deriving Theorem 4.2 are recalled below and a complete proof can be found in [22].

For simplicity, we are going to focus on one of the position coordinates, say the one along the axis  $e_1$ , and derive the invariance principle in this case. From Proposition 4.1, the operator  $\mathcal{L}$  is invertible on the space  $\mathbb{L}^2(M_\beta)$  of functions of mean 0, thus there exists a unique solution to the Poisson equation associated with the velocity

$$-\mathcal{L}\psi(v) = v_{e_1} \quad \text{with} \quad \mathbb{E}_{M_\beta}(\psi) = 0. \quad (4.16)$$

The stochastic process

$$\mathcal{M}_t = \psi(v(t)) - \psi(v(0)) - \alpha \int_0^t ds \mathcal{L}\psi(v(s))$$

is a martingale. Since  $\psi$  is a solution of the Poisson equation, the invariance principle for the position  $x_{e_1}(\alpha\tau)$  will be deduced from the invariance principle for the martingale  $\tau \rightarrow \mathcal{M}_{\alpha\tau}$

$$x_{e_1}(\alpha\tau) = \int_0^{\alpha\tau} ds v_{e_1}(s) = \frac{1}{\alpha} \mathcal{M}_{\alpha\tau} - \frac{1}{\alpha} (\psi(v(\alpha\tau)) - \psi(v(0))). \quad (4.17)$$

Indeed, the second term can be neglected as it converges to 0 in  $\mathbb{L}^2$  by (4.16)

$$\frac{1}{\alpha^2} \mathbb{E}_{M_\beta}(\psi^2) = \frac{1}{\alpha^2} \mathbb{E}_{M_\beta} \left( \left( \mathcal{L}^{-1} v_{e_1} \right)^2 \right) \xrightarrow{\alpha \rightarrow \infty} 0.$$

The inequality

$$\forall r \in \mathbb{R}, \quad |\exp(ir) - 1 - ir| \leq r^2$$

implies that the characteristic function of  $x_{e_1}(\alpha\tau)$  is well approximated by the one of  $\frac{1}{\alpha} \mathcal{M}_{\alpha\tau}$ .

The square of the martingale can be decomposed as

$$\mathcal{M}_t^2 = \alpha \int_0^t ds \left( \mathcal{L}\psi^2(v(s)) - 2\psi(v(s))\mathcal{L}\psi(v(s)) \right) + N_t,$$

where  $N_t$  is another martingale. Thus the variance (4.11) can be recovered by computing the variance of the martingale term in (4.17)

$$\mathbb{E}_{M_\beta} \left( \frac{\mathcal{M}_{\alpha\tau}^2}{\alpha^2} \right) = -2 \frac{\alpha^2 \tau}{\alpha^2} \mathbb{E}_{M_\beta} (\psi \mathcal{L} \psi) = 2\tau \mathbb{E}_{M_\beta} (v_{e_1} (-\mathcal{L})^{-1} v_{e_1}) = 2\mathbf{D}\tau, \quad (4.18)$$

where we used (4.16) in the last equality. More precisely, the ergodic theorem implies the convergence of the quadratic variation almost surely and in  $\mathbb{L}^1(M_\beta)$

$$\frac{1}{\alpha} \int_0^{\alpha\tau} ds (\mathcal{L}\psi^2 - 2\psi\mathcal{L}\psi)(v(s)) = \frac{1}{\alpha} \int_0^{\alpha\tau} ds (\mathcal{L}(\mathcal{L}^{-1}v_{e_1})^2 - 2v_{e_1}\mathcal{L}^{-1}v_{e_1})(v(s)) \xrightarrow[\alpha \rightarrow \infty]{\mathbb{L}^1} 2\mathbf{D}\tau.$$

Thus the assumptions of Theorem 2.1 in [22] are satisfied and this leads to the convergence in law of  $x_{e_1}(\alpha\tau)$  to a Gaussian variable. A similar approach (see Theorem 2.32 in [22]) can be implemented to derive the joint convergence in law (4.14) of the marginals.

It remains to justify the tightness criterion (4.15) which will be a consequence of the following lemma.

**Lemma 4.3.** *Fix  $\eta > 0$  then*

$$\mathbb{E}_{M_\beta} \left( \sup_{0 < \sigma < \eta} \left( \int_0^{\alpha\sigma} v_{e_1}(s) ds \right)^2 \right) \leq 18\eta \mathbb{E}_{M_\beta} (v_{e_1} (-\mathcal{L})^{-1} v_{e_1}).$$

This is Lemma 2.4 from [22] and its proof is derived at the end of this section for the sake of completeness. As the measure  $M_\beta$  is invariant, it is enough to prove (4.15) for  $\tau = 0$ . Lemma 4.3 implies a uniform upper bound in  $\alpha$

$$\mathbb{P}_{M_\beta} \left( \sup_{0 < \sigma < \eta} \left| \int_0^{\alpha\sigma} v_{e_1}(s) ds \right| \geq \delta \right) \leq \frac{18\eta}{\delta^2} \mathbb{E}_{M_\beta} (v_{e_1} (-\mathcal{L})^{-1} v_{e_1}). \quad (4.19)$$

Letting  $\eta$  tend to 0, this completes (4.15) for the coordinate  $v_{e_1}$ . By symmetry of the coordinates of the velocity, the tightness criterion (4.15) follows.

*Proof of Lemma 4.3.* Recall that in (4.17), the additive process has been rewritten in terms of a martingale

$$\alpha \int_0^{\alpha\sigma} v_{e_1}(s) ds = \mathcal{M}_{\alpha\tau} - (\psi(v(\alpha\sigma)) - \psi(v(0))),$$

and the martingale fluctuations can be estimated by Doob's Theorem. To control the fluctuations of the second term with  $\psi$ , we are going also to replace it by a martingale.

Let  $T = \alpha\eta$  and define the backward filtration  $\{\mathcal{F}_t^-; t \in [0, T]\}$  generated by the backward process  $\{v(T-t); t \in [0, T]\}$ . The Markov chain is reversible, so that the generator of the backward process is also  $\alpha\mathcal{L}$ . Thus the following process is also a martingale

$$\mathcal{M}_t^- = \psi(v(T-t)) - \psi(v(T)) - \alpha \int_0^t \mathcal{L}\psi(v(T-s)) ds.$$

In particular, using the Poisson equation (4.16), we get

$$\mathcal{M}_{\alpha\eta}^- - \mathcal{M}_{\alpha(\eta-\sigma)}^- = \psi(v(0)) - \psi(v(\alpha\sigma)) + \alpha \int_0^{\alpha\sigma} v_{e_1}(s) ds.$$

Combined with (4.17), we deduce that

$$2\alpha \int_0^{\alpha\sigma} v_{e_1}(s) ds = \mathcal{M}_{\alpha\sigma} + \mathcal{M}_{\alpha\eta}^- - \mathcal{M}_{\alpha(\eta-\sigma)}^-.$$

Thus the derivation of Lemma 4.3 boils down to controlling the martingale fluctuations by Doob's inequality

$$\begin{aligned} & \mathbb{E}_{M_\beta} \left( \sup_{0 < \sigma < \eta} \left( \int_0^{\alpha\sigma} v_{e_1}(s) ds \right)^2 \right) \\ &= \frac{3}{4\alpha^2} \left( \mathbb{E}_{M_\beta} \left( \sup_{0 < \sigma < \eta} \mathcal{M}_{\alpha\sigma}^2 \right) + \mathbb{E}_{M_\beta} \left( \sup_{0 < \sigma < \eta} (\mathcal{M}_{\alpha(\eta-\sigma)}^-)^2 \right) + \mathbb{E}_{M_\beta} \left( (\mathcal{M}_{\alpha\eta}^-)^2 \right) \right) \\ &\leq \frac{3}{\alpha^2} \left( \mathbb{E}_{M_\beta} \left( \mathcal{M}_{\alpha\eta}^2 \right) + 2\mathbb{E}_{M_\beta} \left( (\mathcal{M}_{\alpha\eta}^-)^2 \right) \right) = 18\eta \mathbb{E}_{M_\beta} \left( v_{e_1}(-\mathcal{L})^{-1} v_{e_1} \right), \end{aligned}$$

where we used the computation (4.18) of the variance.  $\square$

### 4.3 Hard-sphere dynamics

We are going to study the asymptotic behavior of a tagged particle in the hard-sphere dynamics at equilibrium and show that after rescaling its trajectory converges to a Brownian motion.

#### 4.3.1 The convergence result

In the hard-sphere gas, all the particles are exchangeable and we are going to break this symmetry in order to follow the evolution of a given particle which will play a specific role. This tagged particle will be labelled by 1 with coordinates  $z_1 = (x_1, v_1)$ . The initial data is a perturbation of the equilibrium density (2.18) with respect to the position  $x_1$  of the tagged particle

$$\forall Z_N \in \mathbb{D}_\varepsilon^N, \quad f_N(0, Z_N) := \rho^0(x_1) M_{N,\beta}(Z_N), \quad (4.20)$$

where  $\rho^0 \in C^0(\mathbb{T}^d)$  is a continuous density of probability on  $\mathbb{T}^d$ . Note that the distribution  $f_N(0)$  is normalized by 1 in  $\mathbb{L}^1(\mathbb{T}^{dN} \times \mathbb{R}^{dN})$  thanks to the translation invariance of  $\mathbb{T}^d$  and that  $\int_{\mathbb{T}^d} \rho^0(x) dx = 1$ .

In the macroscopic limit  $\alpha \rightarrow \infty$ , the trajectory of the tagged particle is rescaled as

$$\widehat{\chi}_\alpha(\tau) := x_1(\alpha\tau) \in \mathbb{T}^d, \quad (4.21)$$

where  $\tau$  stands for the macroscopic time scale. The distribution of  $\widehat{\chi}_\alpha(\tau)$  is given by the first marginal  $f_N^{(1)}(\alpha\tau, x, v)$  of the particle system. The following theorem, derived in [6], describes the macroscopic behavior of the tagged particle and of its density.

**Theorem 4.4.** *Consider a tagged particle in a hard-sphere gas initially distributed according to the density defined in (4.20). Then, in the limit*

$$N \rightarrow \infty, \quad \varepsilon \rightarrow 0, \quad \alpha \rightarrow \infty \quad \text{with} \quad \alpha = N\varepsilon^{d-1} \quad \text{and} \quad \alpha \ll \sqrt{\log \log N}, \quad (4.22)$$

the process  $\{\widehat{\chi}_\alpha(\tau)\}_{\tau \geq 0}$  associated with the tagged particle (4.21) converges in law towards a Brownian motion initially distributed under the measure  $\rho^0$  and with variance  $2\mathbf{D}$  given by (4.10).

In particular, the distribution  $f_N^{(1)}(\alpha\tau, x, v)$  of  $\widehat{\chi}_\alpha(\tau)$  is well approximated, in the limit (4.22), by

$$\|f_N^{(1)}(\alpha\tau, x, v) - \rho(\tau, x)M_\beta(v)\|_{\mathbb{L}^\infty([0, T] \times \mathbb{T}^d \times \mathbb{R}^d)} \rightarrow 0, \quad (4.23)$$

where  $\rho(\tau, x)$  is the solution of the linear heat equation

$$\partial_\tau \rho - \mathbf{D}\Delta_x \rho = 0 \quad \text{in} \quad \mathbb{T}^d \quad \text{with} \quad \rho|_{\tau=0} = \rho^0. \quad (4.24)$$

The heat equation should be understood as a (simple) hydrodynamic limit because it arises in a regime such that the tagged particle undergoes a diverging number of collisions per unit time. The derivation of this hydrodynamic equation relies on the kinetic approximation of the microscopic dynamics, however contrary to the strategy described in Section 1.3, the hydrodynamic equation is not obtained in a two-step limit but in the joint limit  $N, \alpha \rightarrow \infty$  (4.22).

The invariance principle will be proved by coupling the process  $\{\widehat{\chi}_\alpha(\tau)\}_{\tau \geq 0}$  with the rescaled Markov chain  $\{\widehat{\chi}_\alpha(\tau)\}_{\tau \geq 0}$  introduced in (4.9). The probability that both processes coincide in the coupling is shown to converge to 1 with an explicit error depending on  $N, \varepsilon, \alpha$ . Then the invariance principle for the Markov chain (Theorem 4.2) implies, in the limit (4.22), the convergence of the tagged particle in the mechanical process to a Brownian motion. The following theorem is a simplified version of this coupling showing that the distance between the densities at time  $t$  of both processes can be estimated quantitatively in terms of  $N, \alpha, t$ .

**Theorem 4.5.** *The distribution  $f_N^{(1)}(t, x, v)$  of the tagged particle is close to  $M_\beta(v)\varphi_\alpha(t, x, v)$ , where  $\varphi_\alpha(t, x, v)$  is the solution of the linear Boltzmann equation (4.8) with initial data  $\rho^0$ . More precisely, for all  $t > 0$  and all  $\alpha > 1$ , in the limit  $N \rightarrow \infty$ , with  $N\varepsilon^{d-1} = \alpha$ , one has*

$$\|f_N^{(1)}(t, x, v) - M_\beta(v)\varphi_\alpha(t, x, v)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C \left[ \frac{t\alpha}{(\log \log N)^{\frac{A-1}{A}}} \right]^{\frac{A^2}{A-1}}, \quad (4.25)$$

where  $A \geq 2$  can be taken arbitrarily large, and  $C$  depends on  $A, \beta, d$  and  $\|\rho^0\|_{\mathbb{L}^\infty}$ .

The coupling of the full trajectories is postponed to Section .....

In [47, 24], van Beijeren, Lanford, Lebowitz and Spohn derived the linear Boltzmann equation for any time  $t > 0$  (independent of  $N$ ). Theorem 4.5 is an enhanced result which provides quantitative estimates on the convergence up to times diverging when  $N \rightarrow \infty$ . The coupling between the measures on the trajectories is postponed to Section 4.3.8.

### 4.3.2 BBGKY and Boltzmann hierarchies

The BBGKY and Boltzmann hierarchies can be defined as in Section 3.2. However, contrary to the derivation of the Boltzmann equation, the symmetry of the labels is broken as the first particle is tagged and therefore plays a specific role. The coordinates of the other particles in the gas are symmetric. We briefly recall the definition of the hierarchies in this modified framework and stress the new features.

Using the notation of Proposition 3.2, the marginals of the hard-sphere dynamics are given by

$$\forall s \leq N, \quad f_N^{(s)}(t) = \sum_{n=0}^{N-s} \alpha^n Q_{s,s+n}(t) f_N^{(s+n)}(0), \quad (4.26)$$

where the initial data was introduced in (4.20)

$$\forall Z_N \in \mathcal{D}_\varepsilon^N, \quad f_N(0, Z_N) = \rho^0(x_1) M_{N,\beta}(Z_N).$$

As the initial data is a perturbation of the stationary measure, uniform estimates in time can be derived on the marginals.

**Proposition 4.6.** *For any  $s \geq 1$ , the following bound holds uniformly with respect to time for almost all configurations  $Z_s$  in  $\mathbb{T}^{sd} \times \mathbb{R}^{sd}$*

$$\sup_{t \geq 0} \left| f_N^{(s)}(t, Z_s) \right| \leq \|\rho^0\|_{\mathbb{L}^\infty(\mathbb{T}^d)} M_{N,\beta}^{(s)}(Z_s) \leq C^s \|\rho^0\|_{\mathbb{L}^\infty(\mathbb{T}^d)} M_\beta^{\otimes s}(V_s), \quad (4.27)$$

for some  $C > 0$  depending on  $\beta$  and  $d$ , provided that  $\alpha\varepsilon \ll 1$ .

As a consequence, the weighted norms (3.29) are uniformly controlled in time

$$\forall s \leq N, \quad \sup_{t \geq 0} \|f_N^{(s)}(t)\|_{\varepsilon,s,\beta} \leq C^s \|\rho^0\|_{\mathbb{L}^\infty(\mathbb{T}^d)}, \quad (4.28)$$

for some constant  $C > 0$ .

These estimates will play a crucial role to control the collision operators as they imply that particles are not clustering so that the collision frequency remains controlled in time.

*Proof.* By definition of the initial data (4.20), the following bound holds

$$f_N(0, Z_N) = \rho^0(x_1) M_{N,\beta}(Z_N) \leq \|\rho^0\|_{\mathbb{L}^\infty} M_{N,\beta}(Z_N).$$

As  $M_{N,\beta}$  is a stationary solution of the Liouville equation (see Proposition 2.3), the maximum principle derived in Proposition 2.2 implies that

$$\forall t \geq 0, \quad f_N(t, Z_N) \leq \|\rho^0\|_{\mathbb{L}^\infty} M_{N,\beta}(Z_N).$$

The inequalities for the marginals follow by integration for any  $s \leq N$

$$\forall t \geq 0, \quad f_N^{(s)}(t, Z_s) \leq M_{N,\beta}^{(s)}(Z_s) \|\rho^0\|_{\mathbb{L}^\infty}.$$

The last inequality in (4.27) is a consequence of Proposition 2.4, provided that  $\alpha\varepsilon \ll 1$ .

Combining (4.27) and Definition (3.29) of the weighted norms, we get

$$\|f_N^{(s)}(t)\|_{\varepsilon,s,\beta} \leq C^s \|\rho^0\|_{\mathbb{L}^\infty} \left\| M_\beta^{\otimes s}(V_s) \exp(\beta H_s(Z_s)) \right\|_{\mathbb{L}^\infty(\mathbb{D}_\varepsilon^s)}.$$

This completes (4.28).  $\square$

The limiting Boltzmann hierarchy is defined, as in (3.17), by

$$\forall s \geq 1, \quad \partial_t g_\alpha^{(s)} + \sum_{i=1}^s v_i \cdot \nabla_{x_i} g_\alpha^{(s)} = \alpha C_{s,s+1}^0 g_\alpha^{(s+1)},$$

with the initial data

$$g_\alpha^{(s)}(0, Z_s) = \rho^0(x_1) M_\beta^{\otimes s}(V_s). \quad (4.29)$$

The solution of the Boltzmann hierarchy is explicit and it is related to the density of a tagged particle in an ideal gas at equilibrium (4.8).

**Lemma 4.7.** *Let  $\varphi_\alpha(t, z)$  be the solution of the linear Boltzmann equation (4.8) with initial data  $\varphi_\alpha(0, z) = \rho^0(x)$ . Then the unique solution of the Boltzmann hierarchy starting from the initial data (4.29) is given by*

$$\forall s \geq 1, \quad g_\alpha^{(s)}(t, Z_s) = \varphi_\alpha(t, z_1) M_\beta^{\otimes s}(V_s). \quad (4.30)$$

In particular, this solution satisfies the uniform bound

$$\forall s \geq 1, \quad \sup_{t \geq 0} \|g_\alpha^{(s)}(t)\|_{0,s,\beta} \leq C^s \|\rho^0\|_{L^\infty}, \quad (4.31)$$

where the constant  $C$  depends only on  $\beta$  and  $d$ .

*Proof.* Plugging (4.30) in the Boltzmann hierarchy implies the existence of a solution. Uniqueness follows from Proposition 3.7. The uniform bound is a consequence of the maximum principle for the linear Boltzmann equation (4.8).  $\square$

We stress the fact that the solution (4.30) of Boltzmann hierarchy depends on the structure of the initial data and differs from the solution obtained in Lemma 3.3 for symmetric initial data. Finally, the solution (4.30) can be also formulated in terms of the iterated Duhamel formula (3.20)

$$\forall s \geq 1, \quad g_\alpha^{(s)}(t) = \sum_{n \geq 0} \alpha^n Q_{s,s+n}^0(t) g_\alpha^{(s+n)}(0). \quad (4.32)$$

By construction the marginals of the initial data are given by

$$f_N^{(s)}(0, Z_s) := \int f_N(0, Z_N) dz_{s+1} \dots dz_N = \rho^0(x_1) M_{N,\beta}^{(s)}(Z_s).$$

Thus using Proposition 2.7 (or Proposition 2.4), we deduce that the initial data (4.20) and (4.29) are close in the following sense.

**Proposition 4.8.** *There is a constant  $C > 0$  such that, in the scaling  $N\varepsilon^{d-1} = \alpha \ll 1/\varepsilon$ , the following holds uniformly in  $N$*

$$s \leq N, \quad \left| \left( f_N^{(s)}(0, Z_s) - g_\alpha^{(s)}(0, Z_s) \right) \mathbf{1}_{\mathbb{D}_\varepsilon^s}(Z_s) \right| \leq C^s \varepsilon \alpha \|\rho^0\|_{\mathbb{L}^\infty} M_\beta^{\otimes s}(V_s).$$

### 4.3.3 The pruning procedure

Let us fix a (small) parameter  $h > 0$  and a sequence  $\{n_k\}_{k \geq 1}$  of integers to be tuned later. We shall study the dynamics up to time  $t := Kh$  for some large integer  $K$ , by splitting the time interval  $[0, t]$  into  $K$  intervals, and controlling the number of collisions on each interval. In order to discard trajectories with a large number of collisions in the iterated Duhamel formula (4.26), we define *good* collision trees by the condition that they have strictly less than  $n_k$  collisions on the interval  $[t - kh, t - (k - 1)h]$ .

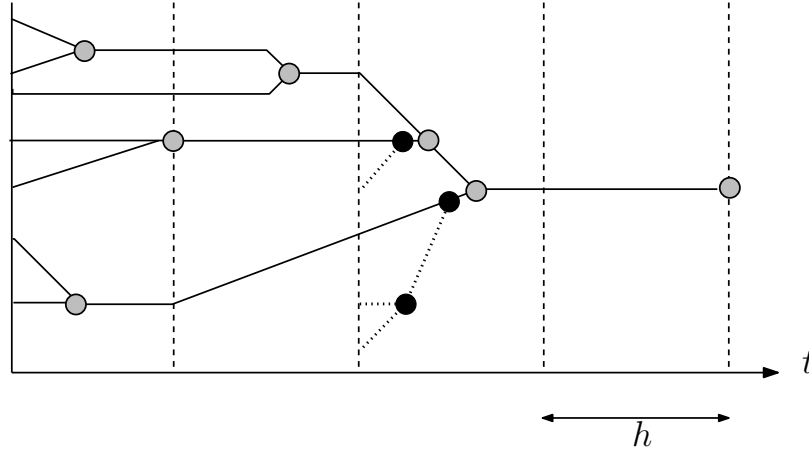


Figure 4.2: Suppose  $n_k = A^k$  with  $A = 2$ . Each collision is represented by a circle from which 2 trajectories emerge. The tree including the three extra collisions in dotted lines occurring during  $[t - 2h, t - h]$  is not a good collision tree and in our procedure, it would be truncated at time  $t - 2h$ . The tree without the dotted lines is a good collision tree with  $t = 4h$ : the number of collisions during the  $k^{\text{th}}$ -time interval is less than  $n_k - 1 = A^k - 1$ .

We start by using (4.26) with  $s = 1$ , during the time interval  $[t - h, t]$ : iterating Duhamel's formula up to time  $t - h$  instead of time 0, we have

$$f_N^{(1)}(t) = \sum_{j_1=0}^{n_1-1} \alpha^{j_1-1} Q_{1,1+j_1}(h) f_N^{(j_1)}(t-h) + R_{1,n_1}(t-h, t), \quad (4.33)$$

where  $R_{1,n_1}(t', t)$  accounts for at least  $n_1$  collisions in the time interval  $[t', t]$

$$R_{1,n_1}(t', t) := \sum_{\ell=n_1}^{N-1} \alpha^\ell Q_{1,\ell+1}(t-t') f_N^{(\ell+1)}(t').$$

More generally, we define  $R_{k,n}$  as follows

$$R_{k,n}(t', t) := \sum_{\ell=n}^{N-k} \alpha^\ell Q_{k,k+\ell}(t-t') f_N^{(k+\ell)}(t'). \quad (4.34)$$

The term  $R_{k,n}(t', t)$  accounts for trajectories with  $k$  particles at time  $t$ , and involving at least  $n$  collisions during the time-span  $t - t'$ . If  $t - t'$  is small then it is atypical to have a large number of collisions, thus  $R_{k,n}(t', t)$  should be negligible for  $n$  large.

The first term on the right-hand side of (4.33) can be decomposed again by iterating the Duhamel formula on the time interval  $[t - 2h, t - h]$  and truncating the contributions with more than  $n_2$  collisions:

$$\begin{aligned} f_N^{(1)}(t) &= \sum_{j_1=0}^{n_1-1} \sum_{j_2=0}^{n_2-1} \alpha^{j_1+j_2} Q_{1,1+j_1}(h) Q_{1+j_1,1+j_1+j_2}(h) f_N^{(1+j_1+j_2)}(t-2h) \\ &\quad + R_{1,n_1}(t-h, t) + \sum_{j_1=0}^{n_1-1} \alpha^{j_1} Q_{1,j_1+1}(h) R_{j_1+1,n_2}(t-2h, t-h). \end{aligned}$$

Iterating this procedure  $K$  times and truncating the trajectories with at least  $n_k$  collisions during the time interval  $[t - kh, t - (k-1)h]$ , leads to the following expansion

$$f_N^{(1)}(t) = f_N^{(1,K)}(t) + R_N^K(t), \quad (4.35)$$

with the notation  $J_0 := 1$  and  $J_k := 1 + j_1 + \dots + j_k$ ,

$$f_N^{(1,K)}(t) := \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} \alpha^{J_K-1} Q_{1,J_1}(h) Q_{J_1,J_2}(h) \dots Q_{J_{K-1},J_K}(h) f_N^{(J_K)}(0) \quad (4.36)$$

and

$$R_N^K(t) := \sum_{k=1}^K \sum_{j_1=0}^{n_1-1} \dots \sum_{j_{k-1}=0}^{n_{k-1}-1} \alpha^{J_{k-1}-1} Q_{1,J_1}(h) \dots Q_{J_{k-2},J_{k-1}}(h) R_{J_{k-1},n_k}(t - kh, t - (k-1)h),$$

where the last term was introduced in (4.34). By an appropriate choice of the sequence  $\{n_k\}_{k \geq 1}$ , we are going to show that the main contribution to the density  $f_N^{(1)}(t)$  is given by  $f_N^{(1,K)}(t)$  and that the remainder  $R_N^K(t)$  vanishes asymptotically.

The solution of the Boltzmann hierarchy defined in (4.32) can also be truncated as in (4.36).

$$g_\alpha^{(1)}(t) = g_\alpha^{(1,K)}(t) + R_\alpha^K(t), \quad (4.37)$$

where

$$g_\alpha^{(1,K)}(t) := \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} \alpha^{J_K-1} Q_{1,J_1}^0(h) Q_{J_1,J_2}^0(h) \dots Q_{J_{K-1},J_K}^0(h) g_\alpha^{(J_K)}(0) \quad (4.38)$$

and

$$R_\alpha^K(t) := \sum_{k=1}^K \sum_{j_1=0}^{n_1-1} \dots \sum_{j_{k-1}=0}^{n_{k-1}-1} \alpha^{J_{k-1}-1} Q_{1,J_1}^0(h) \dots Q_{J_{k-2},J_{k-1}}^0(h) R_{J_{k-1},n_k}^0(t - kh, t - (k-1)h)$$

with

$$R_{k,n}^0(t', t) := \sum_{\ell \geq n} \alpha^\ell Q_{k,k+\ell}^0(t-t') g_\alpha^{(k+\ell)}(t').$$

Since the particles undergo on average one collision per unit time, the growth of collision trees is typically exponential. Pathological trees are therefore those with super-exponential growth.



**Proposition 4.9.** *Let  $A \geq 2$  be given and define  $n_k := A^k$ , for  $k \geq 1$ . Then there exist  $c, C, \gamma_0 > 0$  depending on  $d, A$  and  $\beta$  such that for any  $t > 1$  and any  $\gamma \leq \gamma_0$ , choosing*

$$h \leq \frac{c\gamma}{\alpha^{A/(A-1)} t^{1/(A-1)}} \quad \text{and} \quad K = \frac{t}{h} \quad \text{an integer,} \quad (4.39)$$

we get

$$\left\| R_N^K(t) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} + \left\| R_\alpha^K(t) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C\gamma^A \|\rho^0\|_{\mathbb{L}^\infty(\mathbb{T}^d)}. \quad (4.40)$$

*Proof.* We are going to bound each term in the remainder  $R_N^K$ . The occurrence of a large number of collisions in the time interval  $[t - kh, t - (k - 1)h]$  can be estimated from above by neglecting the precise distribution of the collisions in the time interval  $[t - kh, t]$

$$\begin{aligned} & \left\| Q_{1,J_1}(h) \dots Q_{J_{k-2},J_{k-1}}(h) R_{J_{k-1},n_k}(t - kh, t - (k - 1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq \left\| |Q|_{1,J_{k-1}}((k - 1)h) R_{J_{k-1},n_k}(t - kh, t - (k - 1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)}, \end{aligned}$$

where the operator  $|Q|$  was defined in (3.30).

Applying Proposition 3.4, one has

$$\begin{aligned} & \left\| |Q|_{1,J_{k-1}}((k - 1)h) R_{J_{k-1},n_k}(t - kh, t - (k - 1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq \left( \frac{C(k - 1)h}{\beta^{(d+1)/2}} \right)^{J_{k-1}-1} \left\| R_{J_{k-1},n_k}(t - kh, t - (k - 1)h) \right\|_{\varepsilon, J_{k-1}, \beta/2}. \end{aligned} \quad (4.41)$$

Each term in the remainder  $R_{J_{k-1},n_k}$  can be also estimated by Proposition 3.4. For any  $\ell \geq n_k$ , one has

$$\left\| \alpha^\ell Q_{J_{k-1}, J_{k-1}+\ell}(h) f_N^{(J_{k-1}+\ell)}(t - kh) \right\|_{\varepsilon, J_{k-1}, \beta/2} \leq \left( \frac{C\alpha h}{\beta^{(d+1)/2}} \right)^\ell \left\| f_N^{(J_{k-1}+\ell)}(t - kh) \right\|_{\varepsilon, J_{k-1}+\ell, \beta}.$$

The key of the proof is to use the estimate on the marginals (4.28) which holds uniformly in time so that

$$\left\| \alpha^\ell Q_{J_{k-1}, J_{k-1}+\ell}(h) f_N^{(J_{k-1}+\ell)}(t - kh) \right\|_{\varepsilon, J_{k-1}, \beta/2} \leq \left( \frac{C\alpha h}{\beta^{(d+1)/2}} \right)^\ell c^{J_{k-1}+\ell} \|\rho^0\|_{\mathbb{L}^\infty}.$$

The notation  $c$  refers to a constant depending only on  $d$  and  $\beta$ . The parameter  $h$  will be chosen small enough so that the upper bound tends to 0 exponentially fast when  $\ell$  diverges. Plugging this upper bound in (4.41) and renaming the constants, one can write

$$\begin{aligned} & \alpha^{J_{k-1}-1} \left\| |Q|_{1,J_{k-1}}((k - 1)h) R_{J_{k-1},n_k}(t - kh, t - (k - 1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq \|\rho^0\|_{\mathbb{L}^\infty} (C\alpha(k - 1)h)^{J_{k-1}-1} \sum_{\ell=n_k}^{N-J_{k-1}} (C\alpha h)^\ell \\ & \leq \|\rho^0\|_{\mathbb{L}^\infty} (\alpha t)^{J_{k-1}-1} \sum_{\ell=n_k}^{N-J_{k-1}} C^{J_{k-1}+\ell} (\alpha h)^\ell, \end{aligned}$$

where we used that  $(k-1)h \leq t$  and the constant  $C$  depends on  $d, \beta$ . Assuming from now on that

$$h < \frac{1}{2C\alpha}, \quad (4.42)$$

the geometric sum can be bounded by

$$\begin{aligned} \alpha^{J_{k-1}-1} \left\| |Q|_{1, J_{k-1}}((k-1)h) R_{J_{k-1}, n_k}(t - kh, t - (k-1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ \leq 2 \|\rho^0\|_{\mathbb{L}^\infty} (C\alpha t)^{J_{k-1}-1} (C\alpha h)^{n_k}. \end{aligned} \quad (4.43)$$

By definition  $n_j = A^j$ , so that

$$J_{k-1} \leq 1 + n_1 + \dots + n_{k-1} = \frac{A^k - 1}{A - 1} \leq \frac{1}{A - 1} n_k.$$

We deduce that for some constant  $C$

$$\begin{aligned} \alpha^{J_{k-1}-1} \left\| |Q|_{1, J_{k-1}}((k-1)h) R_{J_{k-1}, n_k}(t - kh, t - (k-1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ \leq \exp \left( A^k \left( \log C + \frac{1}{A-1} \log(\alpha t) + \log(\alpha h) \right) \right) \|\rho^0\|_{\mathbb{L}^\infty}. \end{aligned}$$

Therefore, choosing  $h$  as in (4.39), i.e.

$$h \leq \frac{\gamma}{C \alpha^{A/(A-1)} t^{1/(A-1)}},$$

which is compatible with (4.42) as soon as  $\gamma$  is small enough, one has

$$\alpha^{J_{k-1}-1} \left\| |Q|_{1, J_{k-1}}((k-1)h) R_{J_{k-1}, n_k}(t - kh, t - (k-1)h) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq \exp \left( A^k \log \gamma \right) \|\rho^0\|_{\mathbb{L}^\infty}. \quad (4.44)$$

The previous bound is uniform for any collision tree with  $j_i \leq n_i - 1$  up to level  $k-1$ . The number of such sequences  $(j_1, \dots, j_{k-1})$  is bounded by

$$\prod_{i=1}^{k-1} n_i = A^{\frac{k(k-1)}{2}}.$$

The remainder can then be estimated by summing over all the possible choices of  $(j_1, \dots, j_k)$  and using (4.44)

$$\begin{aligned} \left\| R_N^K \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} &\leq \|\rho^0\|_{\mathbb{L}^\infty} \sum_{k=1}^K \exp \left( \frac{k(k-1)}{2} \log(A) + A^k \log \gamma \right) \\ &\leq \|\rho^0\|_{\mathbb{L}^\infty} \sum_{k=1}^K \exp \left( A k \log \gamma \right) \leq C_A \|\rho^0\|_{\mathbb{L}^\infty} \gamma^A, \end{aligned}$$

for  $\gamma$  sufficiently small, where  $C_A$  is a constant depending on  $A$ . Thus, we get the first part of (4.40)

$$\left\| R_N^K \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C \gamma^A \|\rho^0\|_{\mathbb{L}^\infty}. \quad (4.45)$$

A similar argument applies in the case of the Boltzmann hierarchy:

$$\begin{aligned} & \alpha^{J_{k-1}-1} \left\| \left| Q_{1, J_{k-1}}^0((k-1)h) R_{J_{k-1}, n_k}^0(t - kh, t - (k-1)h) \right| \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq (C\alpha t)^{J_{k-1}-1} (C\alpha h)^{n_k} \sup_{t \geq 0} \left\| g_\alpha^{(J_{k-1}+n_k)}(t) \right\|_{0, J_{k-1}+n_k, \beta} \\ & \leq C^{J_{k-1}+n_k} (\alpha t)^{J_{k-1}-1} (\alpha h)^{n_k} \|\rho^0\|_{\mathbb{L}^\infty}, \end{aligned}$$

hence with the choice (4.39) of  $h$ , the same bound as (4.45) holds for the Boltzmann hierarchy

$$\left\| R_\alpha^K \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C \gamma^A \|\rho^0\|_{\mathbb{L}^\infty},$$

Proposition 4.9 is proved.  $\square$

#### 4.3.4 Quantitative estimate of the recollisions

In (4.35) and (4.37), the Duhamel series associated with the first marginal have been decomposed into a main contribution, with collision trees of controlled size, and remainders taking into account very large collision trees

$$f_N^{(1)}(t) = f_N^{(1,K)}(t) + R_N^K(t), \quad g_\alpha^{(1)}(t) = g_\alpha^{(1,K)}(t) + R_\alpha^K(t).$$

The remainders  $R_N^K$  and  $R_\alpha^K$  have been estimated in Proposition 4.9. The next step is to prove the convergence of  $f_N^{(1,K)} - g_\alpha^{(1,K)}$  to 0. The convergence established in Section 3.4.2 is not quantitative and therefore the arguments have to be strengthened in order to control the diverging time scale. We are going to show that

**Proposition 4.10.** *Under the Boltzmann-Grad scaling  $N\varepsilon^{d-1} = \alpha \gg 1$ , we have*

$$\forall t \geq 1, \quad \left\| f_N^{(1,K)}(t) - g_\alpha^{(1,K)}(t) \right\|_{\mathbb{L}^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq \|\rho^0\|_{\mathbb{L}^\infty(\mathbb{T}^d)} (C\alpha t)^{A^{K+1}} \left( \varepsilon |\log \varepsilon|^{d+10} + \frac{\varepsilon}{\alpha} \right). \quad (4.46)$$

Before deriving Proposition 4.10, let us first complete the proof of Theorem 4.5.

To control efficiently the remainders  $R_N^K, R_\alpha^K$  by Proposition 4.9, the sampling time  $h$  has to be chosen small enough. However, the main parts  $f_N^{(1,K)}, g_\alpha^{(1,K)}$  involve trees of size  $A^K$  with  $K = t/h$  so that the estimate (4.46) deteriorates as  $h$  gets too small. The parameters have to be adjusted to optimize these constraints. The upper bound (4.46) imposes that  $(C\alpha t)^{A^{K+1}} \ll \frac{1}{\varepsilon}$  which forces us to choose  $K \ll \frac{\log \log N}{\log A}$ . Once  $K$  is fixed the other parameters introduced in (4.39) can be determined. We set

$$K = \left\lfloor \frac{\log \log N}{2 \log A} \right\rfloor, \quad \gamma = C_1 \frac{(\alpha t)^{\frac{A}{A-1}}}{K} = C \frac{(\alpha t)^{\frac{A}{A-1}}}{\log \log N}, \quad \alpha \ll \frac{1}{\varepsilon}. \quad (4.47)$$

for some constants  $C_1, C$  large enough. Propositions 4.9 and 4.10 imply that for  $t \geq 1$

$$\begin{aligned} & \|f_N^{(1)}(t) - g_\alpha^{(1)}(t)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq \|f_N^{(1,K)}(t) - g_\alpha^{(1,K)}(t)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} + \|R_N^K(t)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} + \|R_\alpha^K(t)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \\ & \leq \exp\left(\log(\alpha t)\sqrt{\log N} + \log \varepsilon\right) + C \left[ \frac{t\alpha}{(\log \log N)^{\frac{A-1}{A}}} \right]^{\frac{A^2}{A-1}}. \end{aligned}$$

Since  $g_\alpha^{(1,K)}(t, z) = M_\beta(v)\varphi_\alpha(t, z)$  by Lemma 4.7, this implies Theorem 4.5.

The main ingredients involved in the derivation of Proposition 4.10 are described below and its proof is postponed to Section 4.3.6. The key step of the proof is Proposition 4.12 where the contribution of the BBGKY pseudo-trajectories with recollisions is shown to be negligible. First of all, the collision trees with large velocities have to be neglected. Define

$$\mathcal{V}_s = \{V_s \in \mathbb{R}^{sd}, \quad |V_s|^2 \leq C_0 |\log \varepsilon|\}, \quad (4.48)$$

for some constant  $C_0$  to be tuned in Lemma 4.11. The pseudo-trajectories with large velocities will be controlled by the terms

$$\begin{aligned} f_N^{(1,K),vel}(t) & := \sum_{j_1=0}^{n_1-1} \dots \sum_{j_k=0}^{n_k-1} Q_{1,J_1}(h) Q_{J_1,J_2}(h) \dots Q_{J_{k-1},J_k}(h) (f_N^{(J_k)}(0) \mathbf{1}_{\mathcal{V}_{J_k}^c}) \\ g_\alpha^{(1,K),vel}(t) & := \sum_{j_1=0}^{n_1-1} \dots \sum_{j_k=0}^{n_k-1} \alpha^{J_k-1} Q_{1,J_1}^0(h) Q_{J_1,J_2}^0(h) \dots Q_{J_{k-1},J_k}^0(h) (g_\alpha^{(J_k)}(0) \mathbf{1}_{\mathcal{V}_{J_k}^c}), \end{aligned}$$

and the following lemma shows that both terms are negligible.

**Lemma 4.11.** *There exists a constant  $C_0 \geq 0$  in the velocity cut-off (4.48) such that*

$$\forall t \geq 0, \quad \left| f_N^{(1,K),vel}(t) \right| + \left| g_\alpha^{(1,K),vel}(t) \right| \leq \varepsilon n_0^K A^{K^2} (C\alpha t)^{A^K} M_{\beta/2}(z_1),$$

with the sequence  $n_k = A^k$ .

Lemma 4.11 will be derived in Section 4.3.6.

The leading part of the tagged particle density is given by the pseudo-trajectories in trees with controlled size and bounded kinetic energy

$$\begin{aligned} \bar{f}_N^{(1,K)}(t) & = f_N^{(1,K)}(t) - f_N^{(1,K),vel}(t) \\ & = \sum_{j_1=0}^{n_1-1} \dots \sum_{j_k=0}^{n_k-1} Q_{1,J_1}(h) Q_{J_1,J_2}(h) \dots Q_{J_{k-1},J_k}(h) (f_N^{(J_k)}(0) \mathbf{1}_{\mathcal{V}_{J_k}}). \end{aligned}$$

Using the geometric interpretation of the collision trees introduced in Section 3.4, this term is further decomposed into two parts

$$\bar{f}_N^{(1,K)}(t) := f_N^{(1,K),0}(t) + f_N^{(1,K),\geq}(t), \quad (4.49)$$

where  $f_N^{(1,K),0}$  is the contribution of the pseudo-trajectories without recollisions and  $f_N^{(1,K),\geq}$  takes into account the pseudo-trajectories with at least one recollision. Following the proof of Proposition 3.8, each term of the series  $f_N^{(1,K),0}(t)$  can be easily compared to the corresponding terms in the Boltzmann hierarchy as in both cases the pseudo-trajectories follow the free transport. The core of the proof of Proposition 4.10 is to obtain an upper bound on the occurrence of recollisions in the pseudo-trajectories and to show that their contribution is negligible.

**Proposition 4.12.** *The contribution of pseudo-trajectories involving at least a recollision is bounded by*

$$\forall t \geq 1, \quad |f_N^{(1,K),\geq}(t, z_1)| \leq (Ct\alpha)^{A^{K+1}} \varepsilon |\log \varepsilon|^{10} M_{\beta/2}(v_1),$$

for some  $C$  depending on  $\beta, d, A$  and  $\|\rho^0\|_{\mathbb{L}^\infty}$ .

Proposition 4.12 is proved in the next section.

### 4.3.5 Proof of Proposition 4.12: a geometric control of recollisions

This section is devoted to the proof of Proposition 4.12. The first part of the argument relies on geometric estimates for the pseudo-trajectories. The strategy is to derive local conditions for the occurrence of a recollision and to show that these conditions can be estimated by integrating out the parameters associated with at most two collisions. Then in a second part, these estimates are combined with the standard continuity estimates on the collision operators to complete Proposition 4.12.

#### 4.3.5.1 A local control on the recollisions.

The collision operator  $Q_{1,1+n}(t)$  can be represented in terms of pseudo-trajectories and we consider a collision tree of height  $n$  with a given branching structure  $\mathbf{a} \in \mathcal{A}_n$ . Suppose that the first recollision occurs between the particles  $i, j$  at a time  $t_{rec}$  then it imposes a strong geometric constraint on the trajectories of  $i, j$  in the time interval  $[t_{rec}, t]$  and in particular, on the collision parameters involved in the deflections of  $i, j$ . Suppose that  $t_{rec}$  belongs to the interval  $]t_{\theta+1}, t_\theta[$  in between two collision times, for some  $\theta$ , we denote by  $t_{1^*}$  the smallest time in  $[t_\theta, t]$  where the trajectories of  $i, j$  were first deflected or created. The collision at time  $t_{1^*}$  provides some degrees of freedom through the collision parameters  $(v_{1^*}, v_{1^*})$  and we are going to analyze the constraints imposed by the recollision on  $(v_{1^*}, v_{1^*})$ . Different scenarios have to be studied.

#### Self-recollision.

Suppose that the collision at time  $t_{1^*}$  involves both particles  $i$  and  $j$ . It is enough to assume, by symmetry, that  $i$  is the parent of  $j = a(i)$  in the tree. A recollision between  $i, j$  may occur due to the periodicity (see Figure 4.3). As  $j$  is created at time  $t_{1^*}$ , the labels  $j = 1^*$  are identified and the corresponding collision parameters are denoted by  $(v_{1^*}, v_{1^*})$ . At the collision time  $t_{1^*}$ , the relative position of the particles is  $x_j = x_i + \varepsilon v_{1^*}$ , thus a recollision at time  $t_{rec} \geq 0$  imposes that there exists  $v_{rec}$  in  $\mathbb{S}^{d-1}$  such that

$$\varepsilon v_{1^*} + (v_i - v_j)(t_{rec} - t_{1^*}) = \varepsilon v_{rec} + q \quad \text{for some } q \in \mathbb{Z}^d \setminus \{0\}, \quad (4.50)$$

where  $v_i, v_j$  stand for the velocities of  $i, j$  after this collision, i.e. at time  $t_{1^*}$ . As the recollision occurs from the periodicity of  $\mathbb{T}^d$ , the parameter  $q$  represents the translates of the unit box. We define below the set of collision parameters such that (4.50) is satisfied

$$\mathcal{R}(\mathbf{a}, i, j) = \left\{ (v_{1^*}, v_{1^*}, \bar{v}_i) \in \mathbb{S}^{d-1} \times \mathbb{B}_R^2, \quad (4.50) \text{ holds for some } t_{rec} \quad (4.51) \right. \\ \left. \text{and some } q \in \mathbb{Z}^d \setminus \{0\} \right\},$$

where  $\bar{v}_i$  stands for the velocity of  $i$  before the collision and the velocities are restricted to the set

$$\mathbb{B}_R = \{v \in \mathbb{R}^d, \quad |v| \leq R\}. \quad (4.52)$$

This cut-off on the velocities comes from the fact that all the velocities of the pseudo-trajectories involved in  $f_N^{(1,K), \geq}$  are bounded by  $R \leq C_0 \log |\varepsilon|$ .

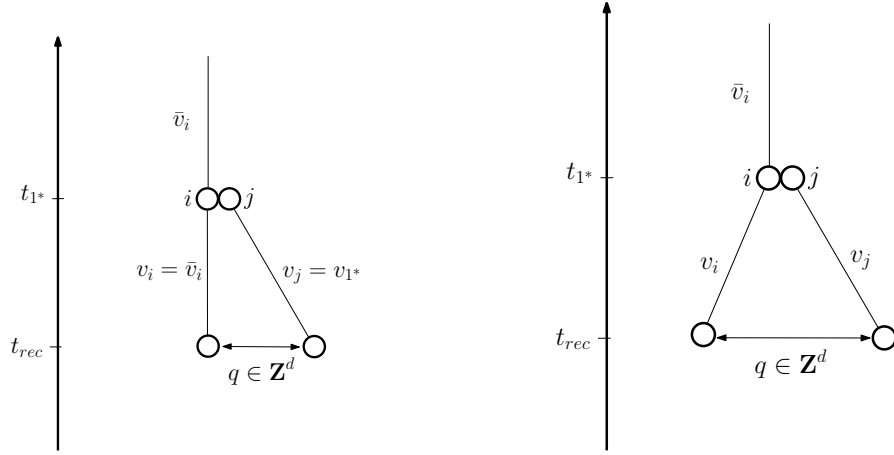


Figure 4.3: A self-recollision between  $i, j$  may happen because of the periodicity of the domain. In both figures, the particle  $j$  is created at time  $t_{1^*}$  from particle  $i$  and  $1^* = j$ . The velocity of  $i$  before the collision is denoted by  $\bar{v}_i$ . On the left figure, the collision is without scattering, instead on the right figure, it is with scattering.

We stress the fact  $\mathcal{R}(\mathbf{a}, i, j)$  encodes a necessary local condition for a self-recollision which is uniform over all the other collision parameters in the tree.

**Lemma 4.13.** *The occurrence of a self-recollision can be bounded from above by*

$$\int \mathbf{1}_{\mathcal{R}(\mathbf{a}, i, j)} |(v_{1^*} - \bar{v}_i) \cdot v_{1^*}| dt_{1^*} dv_{1^*} dv_{1^*} \leq C \varepsilon^{d-1} R^{2d+1} t^{d+1},$$

this holds uniformly for any  $\bar{v}_i \in \mathbb{B}_R$ .

*Proof.* Let us fix  $q \in \mathbb{Z}^d \setminus \{0\}$  and  $t_{1^*} \in [0, t]$ . To compute the measure of the constraint (4.50), two cases have to be distinguished depending on the nature of the collision at  $t_{1^*}$ .

*Collision without scattering.* In this case, the velocity  $v_i = \bar{v}_i$  is unchanged and  $v_j = v_{1^*}$ . Equation (4.50) can be rewritten

$$\bar{v}_i - v_{1^*} = \frac{1}{t_{rec} - t_{1^*}} (q - \varepsilon v_{1^*} + \varepsilon v_{rec}).$$

As the recollision time  $t_{rec}$  is undetermined, this implies that  $v_{1^*} - \bar{v}_i$  belongs to the cone  $\mathbf{C}(q, 2\varepsilon)$  of opening  $\varepsilon$  defined by

$$\mathbf{C}(q, 2\varepsilon) = \{w = u(q + 2\varepsilon v) \in \mathbb{R}^d \text{ for some } u \in \mathbb{R}^+ \text{ and } v \in \mathbb{S}^{d-1}\}.$$

Integrating this constraint over the collision parameters implies that

$$\begin{aligned} \int \mathbf{1}_{\{v_{1^*} - \bar{v}_i \in \mathbf{C}(q, 2\varepsilon) \cap \mathbb{B}_R\}} \left| (v_{1^*} - \bar{v}_i) \cdot v_{1^*} \right| dv_{1^*} dv_{1^*} & \quad (4.53) \\ & \leq CR \int \mathbf{1}_{\{v_{1^*} - \bar{v}_i \in \mathbf{C}(q, 2\varepsilon) \cap \mathbb{B}_R\}} dv_{1^*} dv_{1^*} \leq C\varepsilon^{d-1} R^{d+1}, \end{aligned}$$

where we used that the velocities are bounded by  $R$ .

*Collision with scattering.* Equation (4.50) implies that  $v_i - v_j$  belongs to  $\mathbf{C}(q, 2\varepsilon)$  and the velocities  $v_i, v_j$  after the collision satisfy

$$v_i - v_j = (\bar{v}_i - v_{1^*}) - 2((\bar{v}_i - v_{1^*}) \cdot v_{1^*}) v_{1^*}.$$

Thus for each fixed  $v_{1^*}$ , we conclude that  $\bar{v}_i - v_{1^*}$  is in the cone  $\mathbf{C}_{v_{1^*}}(q, 2\varepsilon)$  (obtained from the cone  $\mathbf{C}(q, 2\varepsilon)$  by symmetry with respect to  $v_{1^*}$ ). As in (4.53), we get by integrating first over  $v_{1^*}$

$$\int \mathbf{1}_{\{v_{1^*} - \bar{v}_i \in \mathbf{C}_{v_{1^*}}(q, 2\varepsilon) \cap \mathbb{B}_{2R}\}} \left| (v_{1^*} - \bar{v}_i) \cdot v_{1^*} \right| dv_{1^*} dv_{1^*} \leq C\varepsilon^{d-1} R^{d+1}. \quad (4.54)$$

To complete Lemma 4.13, we integrate over the collision time  $t_{1^*} \in [0, t]$  which leads to a factor  $t$  as the constraint  $\mathcal{R}(\mathbf{a}, i, j)$  is independent of  $t_{1^*}$  (note that the constraint  $t_{1^*} \geq t_\theta$  has been dropped). Then, it remains to sum over all possible values of  $q$  in the estimates (4.54), (4.53). As the velocities are bounded by  $R$ , the recollision may only occur during  $[0, t]$  at positions such that  $|q| \leq 2Rt + 1$ . This leads to an additional factor  $CR^d t^d$ .  $\square$

### Geometry of the first recollision.

If the collision at time  $t_{1^*}$  does not involve both  $i$  and  $j$ , we may assume, by symmetry, that the collision acts on  $i$ . As previously, several cases have to be considered to take into account that  $i$  may have been deflected or created.

- (i) *Deflection at time  $t_{1^*}$*  : this case is depicted Figure 4.4 (i). Let  $\bar{v}_i$  be the velocity of particle  $i$  before the collision. Then the velocity  $v_i$  after scattering is given by

$$v_i = \bar{v}_i - ((\bar{v}_i - v_{1^*}) \cdot v_{1^*}) v_{1^*}, \quad (i)$$

where  $(v_{1^*}, v_{1^*})$  are the degree of freedom associated with the collision at time  $t_{1^*}$ . In order to gain extra degrees of freedom, we will also consider the collision which occurred before time  $t_{1^*}$ . Let  $t_{2^*} \in ]t_{1^*}, t[$  be the smallest time at which particles  $i$  or  $j$  have been deflected or created. The coordinates of particles  $i, j$  just after the collision at time  $t_{2^*}$  are denoted by  $(\bar{x}_i, \bar{v}_i)$  and  $(x_j, v_j)$ . The condition for the recollision to hold in the backward dynamics at a time  $t_{rec} \geq 0$  then states

$$(\bar{x}_i - x_j) + (t_{1^*} - t_{2^*})(\bar{v}_i - v_j) + (t_{rec} - t_{1^*})(v_i - v_j) = \varepsilon v_{rec} + q, \quad (4.55)$$

for some impact parameter  $v_{rec} \in \mathbb{S}^{d-1}$  and some  $q \in \mathbb{Z}^d$ . The parameter  $q$  takes into account the periodic structure of  $\mathbb{T}^d$ .

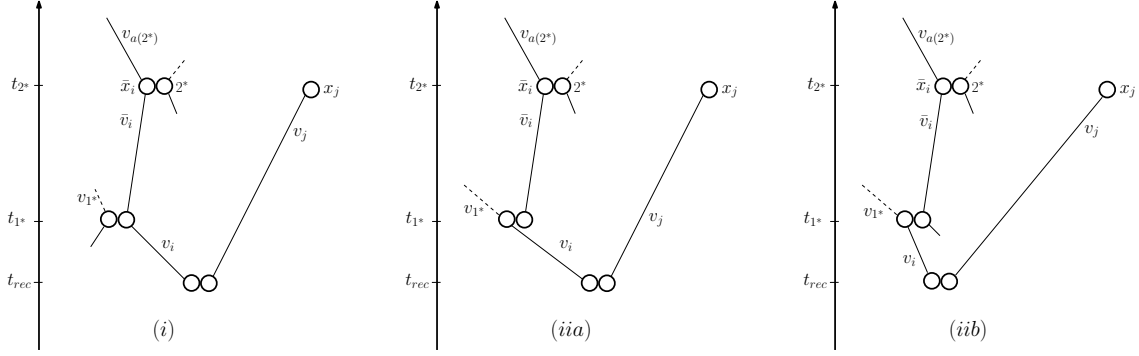


Figure 4.4: The two collisions at times  $t_{1^*}$  and  $t_{2^*}$  leading to the recollision between the pseudo-particles  $i$  and  $j$  are depicted. Three different cases can occur if the first collision involves  $i$ : the particle  $i$  can be deflected (i), created without scattering (iia) or created with scattering (iib). These three cases can also occur for the recollision at  $2^*$  but only one is depicted each time.

- (ii) *Creation at time  $t_{1^*}$* : this leads to the scenarios depicted Figure 4.4 (iia) and (iib). Particle  $i$  coincides with the new particle  $1^*$  and it is created from particle  $a(1^*)$  which has velocity  $\bar{v}_i = v_{a(1^*)}(t_{1^*})$  just before the collision. The velocity of  $i$  after the collision is then given by

$$v_i = v_{1^*}, \quad (\text{iia})$$

if  $(v_{1^*}, v_{1^*}, v_i)$  is a precollisional configuration as on Figure 4.4 (iia) and

$$v_i = v_{1^*} + ((\bar{v}_i - v_{1^*}) \cdot v_{1^*}) v_{1^*}, \quad (\text{iib})$$

if  $(v_{1^*}, v_{1^*}, v_i)$  is a post-collisional configuration as on Figure 4.4 (iib).

We will also consider the collision which occurred just before and denote by  $t_{2^*} \in ]t_{1^*}, t[$  the smallest time at which particles  $a(1^*)$  or  $j$  have been deflected or created (see figure 4.4 (ii)). The coordinates of particles  $a(1^*)$ ,  $j$  just after the collision at time  $t_{2^*}$  are denoted by  $(\bar{x}_i, \bar{v}_i)$  and  $(x_j, v_j)$ . The recollision at time  $t_{rec}$  implies a condition analogous to (4.55)

$$(\bar{x}_i - x_j) + (t_{1^*} - t_{2^*})(\bar{v}_i - v_j) + \varepsilon v_{1^*} + (t_{rec} - t_{1^*})(v_i - v_j) = \varepsilon v_{rec} + q, \quad (4.56)$$

for some impact parameter  $v_{rec} \in \mathbb{S}^{d-1}$  and some  $q \in \mathbb{Z}^d$ . Compared to (4.55), the notation has been chosen so that the only difference is the additional shift  $\varepsilon v_{1^*}$  when particle  $i$  is created.

In all cases, let  $k$  be the label of the particle colliding with  $i$  at time  $t_{1^*}$ :

- in case (i), particle  $k = 1^*$  is created at the collision.
- in cases (iia), (iib), particle  $i = 1^*$  has been created from  $k = a(i)$ .

The label  $1^*$  stands always for the new degrees of freedom associated with this collision. This notation allows us to treat the conditions (4.55) and (4.56) for a recollision in a unified



framework. Consider the set of collision parameters such that

$$\mathcal{R}(a, i, j, k) = \left\{ (t_{1^*}, v_{1^*}, v_{1^*}, \bar{v}_i, v_j, \bar{x}_i, x_j) \in [0, t_{2^*}] \times \mathbb{S}^{d-1} \times \mathbb{B}_R^3 \times \mathbb{T}^{2d}, \right. \quad (4.57)$$

$$\left. (4.55) \text{ or } (4.56) \text{ holds for some } t_{rec} \right\}.$$

Note that  $\mathcal{R}(a, i, j, k)$  encodes a necessary local condition for the recollision which depends only on the collision parameters at time  $t_{1^*}$  and on the coordinates at the collision time  $t_{2^*}$ . The collision at time  $t_{2^*}$  occurs with a new particle and it provides new degrees of freedom denoted by  $v_{2^*}, v_{2^*}$ .

**Lemma 4.14.** *Fix  $1 \leq R^2 \leq C_0 |\log \varepsilon|$  and  $1 \leq t \leq C_0 |\log \varepsilon|$ . In all cases (i), (ia), (ib), the measure of the event  $\mathcal{R}(a, i, j, k)$  is bounded from above by*

$$\int \mathbf{1}_{\mathcal{R}(a, i, j, k)} \prod_{\ell=1^*, 2^*} |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| dt_\ell dv_\ell dv_\ell \leq CR^{2d+2} t^{d+1} \varepsilon |\log \varepsilon|^3, \quad (4.58)$$

uniformly over the coordinates of the pseudo-trajectories at the collision time  $t_2^*$ .

*Proof.* As in the proof of Lemma 4.13, the possible values of  $q$  in (4.55) or (4.56) are such that  $|q| \leq 2Rt + 1$  as the velocities are bounded by  $R$ . Thus it is enough to derive the upper bound (??) for a fixed  $q$  and ultimately to multiply this estimate by  $CR^d t^d$  in order to take into account all the possible values of  $q$ .

### Step 1. Integration of the first collision.

#### 4.3.5.2 Conclusion of the proof of Proposition 4.12

Fix  $z_1 \in \mathbb{T}^d \times \mathbb{B}_R$  with  $R^2 \leq C_0 |\log \varepsilon|$ . In Section 4.3.5.1, a recollision in the pseudo-trajectories was related to local constraints in collision trees. More precisely, given a recollision between  $i, j$  in a tree  $a \in \mathcal{A}_s$ , then two sets of collision parameters  $\mathcal{R}(a, i, j, k)$  and  $\mathcal{R}(\mathbf{a}, i, j)$  have been identified. Given  $a, i, j, k$ , two labels  $1^*$  and  $2^*$  can be uniquely determined and the set  $\mathcal{R}(a, i, j, k)$  imposes restrictions on the corresponding degrees of freedom  $\{t_{\ell^*}, v_{\ell^*}, v_{\ell^*}\}_{\ell=1^*, 2^*}$  (the same is true for  $\mathcal{R}(\mathbf{a}, i, j)$  with only the label  $1^*$ ). By abuse of notation,  $\mathcal{R}(a, i, j, k)$  and  $\mathcal{R}(\mathbf{a}, i, j)$  can be seen as subsets of  $\mathcal{T}_s \times \mathbb{R}^{ds} \times \mathbb{S}^{(d-1)s}$  indexing the whole pseudo-trajectory.

The collision parameters of the pseudo-trajectories with recollision have to belong to

$$\bigcup_{i, j} \mathcal{R}(\mathbf{a}, i, j) \bigcup_{i, j, k} \mathcal{R}(a, i, j, k) \subset \mathcal{T}_s \times \mathbb{R}^{ds} \times \mathbb{S}^{(d-1)s}.$$

Note that the sets  $\mathcal{R}(a, i, j, k)$  and  $\mathcal{R}(\mathbf{a}, i, j)$  are empty if the constraints imposed on the labels  $i, j, k$  and the tree  $a$  cannot be satisfied. Furthermore, the collision parameters in the union above may generate pseudo-trajectories without recollision. Indeed, the sets  $\mathcal{R}(a, i, j, k)$  and  $\mathcal{R}(\mathbf{a}, i, j)$  impose sufficient local conditions at times  $t_{1^*}, t_{2^*}$  for the occurrence of a recollision, but it may happen that the recollision will not take place in the pseudo-trajectory due to the contribution of another collision.

As a consequence,  $f_N^{(1,K), \geq}$  can be bounded from above by

$$\begin{aligned} \left| f_N^{(1,K), \geq}(t, z_1) \right| &\leq \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} \alpha^{J_K-1} \sum_{i,j,k} \sum_{a \in \mathcal{A}_{J_K}} \int_{\mathcal{T}_{2,s}} (\mathbf{1}_{\mathcal{R}(a,i,j,k)} + \mathbf{1}_{\mathcal{R}(a,i,j)}) \\ &\times f_N^{(J_K)}(0, Z_{J_K}) \mathbf{1}_{\mathcal{V}_{J_K}}(Z_{J_K}) \prod_{\ell=1}^{J_K} |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| dt_\ell dv_\ell dv_\ell. \end{aligned} \quad (4.59)$$

In the previous inequality, the constraints on the distribution of the collision times in the different time subintervals of length  $h$  have been neglected.

The following proposition will be the main step to bound  $f_N^{(1,K), \geq}$  from above.

**Proposition 4.15.** *Fix  $z_1 \in \mathbb{T}^d \times \mathbb{R}^d$  as well as the labels  $i, j, k$  in  $\{1, \dots, s\}$ . Then for  $t \geq 1$ , one has*

$$\begin{aligned} \sum_{a \in \mathcal{A}_s} \int_{\mathcal{T}_{2,s}} (\mathbf{1}_{\mathcal{R}(a,i,j,k)} + \mathbf{1}_{\mathcal{R}(a,i,j)}) M_\beta^{\otimes s}(Z_s) \mathbf{1}_{\mathcal{V}_s}(Z_s) \prod_{\ell=1}^s |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| dt_\ell dv_\ell dv_\ell \\ \leq (Ct)^s s^2 \varepsilon |\log \varepsilon|^{d+10} M_{\beta/4}(v_1), \end{aligned} \quad (4.60)$$

where  $Z_s$  stands for the coordinates of the pseudo-trajectory at time 0.

*Proof.* Proposition 4.15 will follow by combining the bounds on the collision operators (see Proposition 3.4) and the local estimates on the recollision derived in Lemmas 4.13 and 4.14. These two types of estimates can be decoupled by using Fubini's theorem and the fact that the sets  $\mathcal{R}(a, i, j)$ ,  $\mathcal{R}(a, i, j, k)$  do not depend on the whole trajectory:  $\mathcal{R}(a, i, j)$  depends only on  $v_{1^*}, v_{1^*}$  and  $\mathcal{R}(a, i, j, k)$  depends on  $\{t_\ell, v_\ell, v_\ell\}_{\ell \in \{1^*, 2^*\}}$  and on the pseudo-trajectory coordinates at the collision time  $t_{2^*}$ . We are simply going to estimate the contribution of  $\mathcal{R}(a, i, j, k)$  as the one of  $\mathcal{R}(a, i, j)$  is simpler.

Given  $a, i, j, k$ , the label  $1^*$  is identified as the degree of freedom occurring in the collision  $i, k$  or  $j, k$ . Then, the label  $2^*$  is determined from the tree  $a$ . By construction particles  $i$  and  $j$  were created before (or at) the collision time  $t_{1^*}$ . Thus the event  $\mathcal{R}(a, i, j, k)$  is independent of the collision parameters larger than  $1^*$ . In order to evaluate (4.60), we first perform the integration with respect to all the velocities and deflection angles with labels larger than  $1^*$  and deduce, from Proposition ??, the following uniform estimates

$$\sum_{(a(k))_{k>1^*}} \left( \prod_{\ell>1^*} |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| \right) M_{\beta/4}^{\otimes s}(V_s) \leq (Cs)^{s-1^*}.$$

Splitting the Maxwellian into two parts, we get by integrating over the labels larger than  $1^*$

$$\sum_{(a(k))_{k>1^*}} \int M_\beta^{\otimes s}(V_s) \prod_{\ell>1^*} |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| dv_\ell dv_\ell \leq (Cs)^{s-1^*} M_{3\beta/4}^{\otimes 1^*}(V_{1^*}). \quad (4.61)$$

This bound takes into account the combinatorics of all the possible branchings for the labels larger than  $1^*$ . In fact, the sum over the trees in (4.60) is restricted to trees compatible with the constraints imposed by the labels  $\{i, j, 1^*, 2^*\}$ , thus (4.61) overestimates the contribution of the labels larger than  $1^*$ .

Recall that the contribution of the collision at time  $t_{1^*}$  has been estimated in (??) uniformly with respect to the pseudo-trajectory coordinates at time  $t_{2^*}$

$$\int \mathbf{1}_{\mathcal{R}(a,i,j,k)} |(v_{1^*} - \bar{v}_i) \cdot v_{1^*}| dt_{1^*} dv_{1^*} \leq C |\log \varepsilon|^{d+1} t^{d+1} \min\left(\frac{\varepsilon}{|\bar{v}_i - v_j|}, 1\right),$$

where the parameter  $R$  is now replaced by  $C_0 |\log \varepsilon|^{d/2}$ . Thus once the integration on the collision at  $t_{1^*}$  has been performed, the integral of the collision parameters for the labels in between  $1^*$  and  $2^*$  can be estimated as in (4.61).

$$\sum_{(a(\ell))_{2^* < \ell < 1^*}} \int \prod_{2^* < \ell < 1^*} |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| M_{3\beta/4}(v_\ell) dv_\ell \leq (Cs)^{1^* - 2^* - 2} M_{\beta/2}^{\otimes 2^*}(V_{2^*}).$$

Once again, this overestimates (4.60) as we are also counting trees for which the branchings in between  $2^*$  and  $1^*$  may not be compatible with the conditions imposed by a recollision.

The previous steps removed all the dependency on the collision trees below the level  $2^*$ . Keeping frozen the parameters of the labels smaller than  $2^*$ , the singularity in (??) can be integrated as in Lemma 4.14, so that we finally get by combining the previous estimates

$$\begin{aligned} \sum_{(a(k))_{k \geq 2^*}} \int M_{3\beta/4}^{\otimes u_1}(V_s) \prod_{\ell=2^*}^s |(v_\ell - v_{a(\ell)}(t_\ell)) \cdot v_\ell| dv_\ell dt_{1^*} dt_{2^*} \\ \leq s(Cs)^{s-2^*-2} t^{d+1} \varepsilon |\log \varepsilon|^{d+4} M_{\beta/2}^{\otimes 2^*-1}(V_{2^*-1}). \end{aligned} \quad (4.62)$$

The additional factor  $s$  in the inequality comes from the choices of  $a(2^*)$ . Note that the time integration has been performed only in  $t_{1^*}, t_{2^*}$ . Once the constraint on the recollision has been taken into account, the remaining part of the tree with the labels less than  $2^*$  can be bounded as in (4.61) by  $(Cs)^{2^*-1}$ .

It remains to integrate over the times  $\{t_i\}_{i \neq 1^*, 2^*}$  under the condition that these  $s-2$  times are ordered. Note that the constraint with respect to  $t_{1^*}, t_{2^*}$  has been already dropped in (4.62). This gives the contribution

$$\frac{t^{s-3}}{(s-3)!} \leq C^s \frac{t^{s-3}}{s^{s-3}},$$

where the upper bound follows from Stirling's formula. This completes the proof of Proposition 4.15.  $\square$

We are now going to complete the proof of Proposition 4.12 and estimate  $f_N^{(1,K), \geq}$  from above. Recall that Proposition 4.6 implies that the marginals of the initial data are dominated by a Maxwellian

$$|f_{N,0}^{(J_K)}(Z_{J_K})| \leq \|\rho^0\|_{L^\infty} C^{J_K} M_\beta^{\otimes J_K}(V_{J_K}).$$

Thus Proposition 4.15 can be used to estimate the integral in (4.59). This leads to

$$\left| f_N^{(1,K), \geq}(t, z_1) \right| \leq \varepsilon |\log \varepsilon|^{d+10} \|\rho^0\|_{L^\infty} \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} \alpha^{J_K-1} (Ct)^{J_K} J_K^5 M_{\beta/4}(v_1),$$

where the sum over the labels  $i, j, k$  in (4.59) has been bounded from above by a factor  $J_K^3$ .

Now recalling that  $n_k = A^k$ , we have

$$J_K \leq A^{K+1} \quad \text{and} \quad \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} \leq \prod_{i=1}^K n_i \leq A^{K^2}. \quad (4.63)$$

We conclude

$$\left| f_N^{(1,K), \geq}(t, z_1) \right| \leq \|\rho^0\|_{L^\infty} A^{4K^2} (Ct\alpha)^{A^{K+1}n_0} \varepsilon |\log \varepsilon|^{d+10} M_{\beta/2}(v_1).$$

Since  $A^{K^2} \ll C^{A^K}$ , this completes the proof of Proposition 4.12.

### 4.3.6 Proof of Proposition 4.10

Each term in the decomposition (4.49)

$$\tilde{f}_N^{(1,K)}(t) = f_N^{(1,K),0}(t) + f_N^{(1,K), \geq}(t)$$

can be interpreted as a restriction of the domain of integration of the times, velocities and deflection angles. For  $f_N^{(1,K), \geq}$ , the pseudo-trajectories associated with a tree  $a$  are integrated over the collision parameters in the set  $\widehat{\mathcal{N}}_\varepsilon(a)$ . The set  $\widehat{\mathcal{N}}_\varepsilon(a)$  plays a role analogous to the one of the set  $\mathcal{N}_\varepsilon$  introduced in (3.61) for the analysis of the recollisions in the derivation of Boltzmann equation. The main difference is that  $\widehat{\mathcal{N}}_\varepsilon(a)$  is not explicit, but its measure, weighted by the product of the cross sections, has been estimated from above in (4.15). In  $f_N^{(1,K),0}$ , the collision parameters are integrated outside  $\widehat{\mathcal{N}}_\varepsilon(a)$  so that the corresponding pseudo-trajectories have no recollisions.

A similar decomposition holds for the Boltzmann hierarchy

$$g_\alpha^{(1,K)}(t) = g_\alpha^{(1,K),0}(t) + g_\alpha^{(1,K), \geq}(t) + g_\alpha^{(1,K), \text{overlap}}(t),$$

where the collision parameters are integrated over different sets : in  $\widehat{\mathcal{N}}_\varepsilon(a)^c \cap G_s(a)$  for  $g_\alpha^{(1,K),0}$ , in  $\widehat{\mathcal{N}}_\varepsilon(a) \cap G_s(a)$  for  $g_\alpha^{(1,K), \geq}(t)$  and finally in  $G_s(a)$  for  $g_\alpha^{(1,K), \text{overlap}}(t)$ . On négligera ce dernier terme.

As a consequence of Proposition 4.12, the term  $\tilde{f}_N^{(1,K), \geq}$  is negligible

$$\left| g_\alpha^{(1,K), \geq}(t, z_1) \right| \leq (CT\alpha)^{A^{K+1}} \varepsilon |\log \varepsilon|^{10} M_{\beta/2}(v_1). \quad (4.64)$$

The last step to conclude Proposition 4.10 is to evaluate the difference  $f_N^{(1,K),0}(t) - g_\alpha^{(1,K),0}(t)$ . Once recollisions and overlaps have been excluded, the only discrepancies between the BBGKY and the Boltzmann pseudo-trajectories come from the micro-translations

due to the diameter  $\varepsilon$  of the colliding particles. At the initial time, the error between the two configurations is at most  $O(s\varepsilon)$  after  $s$  collisions

$$|X_s^0(a, T_{2,s}, \Omega_{2,s}, V_{2,s}, 0) - X_s(a, T_{2,s}, \Omega_{2,s}, V_{2,s}, 0)| \leq C s \varepsilon. \quad (4.65)$$

The discrepancies are only for positions, as velocities remain equal in both hierarchies. These configurations are then evaluated either on the marginals of the initial datum  $f_N^{(s)}(0)$  or of  $g_\alpha^{(s)}(0)$  which are close to each other thanks to Proposition 4.8.

The last source of discrepancy between the formulas defining  $f_N^{(1,K),0}$  and  $g_\alpha^{(1,K),0}$  comes from the prefactor  $(N-1) \dots (N-s+1) \varepsilon^{s-1}$  which has been replaced by  $\alpha^{s-1}$ . For fixed  $s$ , the corresponding error is

$$\left(1 - \frac{(N-1) \dots (N-s+1)}{N^{s-1}}\right) \leq C \frac{s^2}{N} \leq C s^2 \frac{\varepsilon}{\alpha}$$

which, combined with the bound on the collision operators, leads to an error of the form

$$(C\alpha t)^{s-1} s^2 \frac{\varepsilon}{\alpha}. \quad (4.66)$$

Summing the previous bounds gives

$$\begin{aligned} \left|f_N^{(1,K),0}(t, z_1) - \bar{f}^{(1,K),0}(t, z_1)\right| &\leq M_\beta(v_1) \sum_{j_1=0}^{n_1-1} \dots \sum_{j_K=0}^{n_K-1} (C\alpha t)^{J_{k-1}} \left(J_K^2 \frac{\varepsilon}{\alpha} + J_K \varepsilon\right) \\ &\leq M_\beta(v_1) (C T \alpha)^{A^{K+1} n_0} \left(A^{2(K+1)} \frac{\varepsilon}{\alpha} + A^{K+1} \varepsilon\right), \end{aligned} \quad (4.67)$$

where we used the bounds (4.63) for the sequence  $n_k = A^k$ .

Finally Proposition 4.10 follows by combining

- Proposition 4.12 and (4.64) to control the recollisions,
- (4.67) to control the difference in the parts without recollisions.

□

*Proof of Lemma 4.11.* We shall consider only the term from the BBGKY hierarchy as  $g_\alpha^{(1,K),vel}$  can be treated similarly. As the marginals of the initial data can be bounded by a product measure (see for example Proposition 4.6), we get from the tail of the Maxwellian that for  $C_0$  large enough

$$\begin{aligned} \forall s \leq N, \quad \left|f_N^{(s)}(0, Z_s) \mathbf{1}_{\{|V_s|^2 \geq C_0 |\log \varepsilon|\}}\right| &\leq C^s M_\beta^{\otimes s}(V_s) \mathbf{1}_{\{|V_s|^2 \geq C_0 |\log \varepsilon|\}} \|\rho\|_{\mathbb{L}^\infty(\mathbb{T}^d)} \\ &\leq C^s M_{5\beta/6}^{\otimes s}(V_s) \exp\left(-\frac{\beta}{12} |V_s|^2\right) \mathbf{1}_{\{|V_s|^2 \geq C_0 |\log \varepsilon|\}} \\ &\leq \varepsilon C^s M_{5\beta/6}^{\otimes s}(V_s). \end{aligned} \quad (4.68)$$

Neglecting the constraints on the collision time, we get the bound

$$|Q_{1,J_1}(h) Q_{J_1,J_2}(h) \dots Q_{J_{k-1},J_k}(h)| \leq |Q_{1,J_{k-1}}(t),$$

together with the continuity estimates on the collision operators obtained in Proposition 3.4, we deduce from (4.68) that

$$\begin{aligned} & \sum_{k=1}^K \sum_{j_i < n_i} \left| Q_{1,J_1}(h) Q_{J_1,J_2}(h) \cdots Q_{J_{k-1},J_k}(h) (f_N^{(J_k)}(0) \mathbf{1}_{\{|V_{J_k}|^2 \geq C_0 |\log \varepsilon|\}}) \right| \\ & \leq \sum_{k=1}^K \sum_{j_i < n_i} (C\alpha t)^{J_k} \varepsilon M_{\beta/2}(z_1) \leq \varepsilon n_0^K A^{K^2} (C\alpha T)^{A^{K+1}} M_{\beta/2}(z_1). \end{aligned}$$

This concludes the proof of Lemma 4.11.  $\square$

### 4.3.7 Carleman's parametrization and scattering estimates

This final section is devoted to the proof of some technical estimates on the scattering operator used in the derivation of Proposition 4.12.

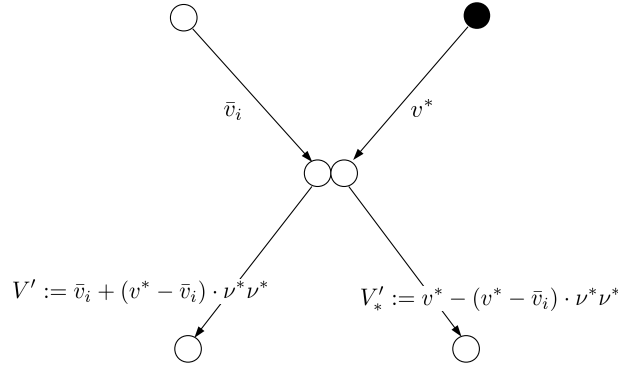


Figure 4.5: Scattering relations.

We introduce the scattering map, known as *Carleman's parametrization*, defined by (see Figure 4.5)

$$(v^*, \nu^*) \in \mathbb{R}^d \times \mathbb{S}^{d-1} \mapsto \begin{cases} V' := \bar{v}_i + ((v^* - \bar{v}_i) \cdot \nu^*) \nu^* \\ V_* := v^* - ((v^* - \bar{v}_i) \cdot \nu^*) \nu^* \end{cases} \quad (4.69)$$

where  $(V', V_*)$  belong to the set

$$\left\{ (V', V_*) \in \mathbb{R}^d \times \mathbb{R}^d, \quad (V' - \bar{v}_i) \cdot (V_* - \bar{v}_i) = 0 \right\}.$$

This map sends the measure  $|((v^* - \bar{v}_i) \cdot \nu^*)| dv^* d\nu^*$  on the measure  $dV' dS(V'_*)$ , where  $dS$  is the Lebesgue measure on the hyperplane  $\mathcal{H}_{V', \bar{v}_i}$  orthogonal to  $(V' - \bar{v}_i)$  and passing through  $\bar{v}_i$ .

**Lemma 4.16.** Fix  $\bar{v}_i$  and  $v_j$  two velocities in  $\mathbb{B}_R = \{v \in \mathbb{R}^d, |v| \leq R\}$ . Given the collision parameters  $(v^*, \nu^*)$ , the velocity  $v_i$  is defined as one of the outgoing velocities  $V'$  or  $V_*$  in (4.69).

Fix  $\delta \in ]0, 1[$ , then the following estimates hold for any  $a \in [1, d - 1]$  uniformly in  $\bar{v}_i, v_j \in \mathbb{B}_R$

$$\int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \mathbf{1}_{\{|v_i - v_j| \leq \delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^d \delta^{d-1} \min\left(\frac{\delta}{|v_j - \bar{v}_i|}, 1\right), \quad (4.70)$$

$$\int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \min\left(\frac{\delta}{|v_i - v_j|}, 1\right) |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^d \delta |\log \delta| + CR^3 \delta^{d-1}, \quad (4.71)$$

where the logarithmic correction occurs only in dimension  $d = 2$ .

*Proof.* We first show Inequality (4.70). Since Carleman's parametrization maps the measure  $|(v^* - \bar{v}_i) \cdot v^*| dv^* dv^*$  on the measure  $dV' dS(V'_*)$ , the size of the event  $\{|V' - v_j| \leq \delta\}$  is of the order  $\delta^d$ . Thus if  $v_i = V'$ , an even better upper bound than (4.70) can be obtained. We turn now to the case  $v_i = V'_*$  which is much more singular as the measure of the event  $\{|V'_* - v_j| \leq \delta\}$  depends on the distance between  $\bar{v}_i$  and  $v_j$ .

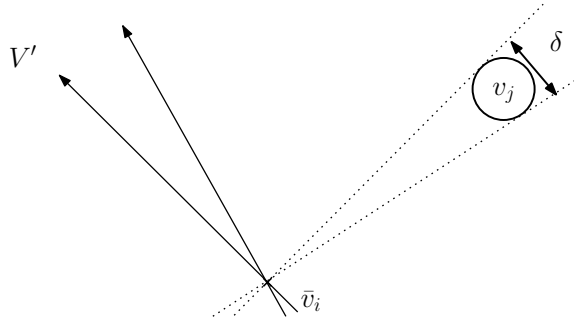


Figure 4.6: Since  $V'_*$  belongs to the ball of radius  $\delta$  around  $v_j$ , it has to be in the cone within the dotted lines. By Carleman's parametrization, this imposes a constraint on the direction of  $V' - \bar{v}_i$ .

If  $|v_j - \bar{v}_i| \leq \delta$ , meaning that  $\bar{v}_i$  is itself in the same ball, then for any  $V' \in \mathbb{B}_R$ , the intersection between the small ball and the hyperplane  $\mathcal{H}_{V', \bar{v}_i}$  has measure at most  $O(\delta^{d-1})$  so that

$$\int \mathbf{1}_{\{|V'_* - v_j| \leq \delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^d \delta^{d-1}.$$

If  $|v_j - \bar{v}_i| > \delta$ , then the intersection between the ball centered at  $v_j$  and the hyperplane  $\mathcal{H}_{V', \bar{v}_i}$  is non empty if the distance between  $v_j$  and  $\mathcal{H}_{V', \bar{v}_i}$  is less than  $\delta$  which implies

$$\left| (v_j - \bar{v}_i) \cdot \frac{V' - \bar{v}_i}{\|V' - \bar{v}_i\|} \right| \leq \delta.$$

Given  $v_j - \bar{v}_i$ , this imposes a constraint on the direction  $V' - \bar{v}_i$  (see Figure 4.6) and this implies

$$\int \mathbf{1}_{\{|V'_* - v_j| \leq \delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^d \delta^{d-1} \frac{\delta}{|v_j - \bar{v}_i|},$$

where  $\delta^{d-1}$  bounds from above the measure of the intersection of the ball with the hyperplane  $\mathcal{H}_{V', \bar{v}_i}$ . Thus (4.70) follows by combining the previous two inequalities.

We turn now to the derivation of Estimate (4.71) which will follow from (4.70) by using Fubini's theorem. We write

$$\begin{aligned} & \int \min\left(\frac{\delta}{|v_i - v_j|}, 1\right) |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ &= \int \mathbf{1}_{\{|v_i - v_j| \leq \delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* + \int \mathbf{1}_{\{|v_i - v_j| > \delta\}} \frac{\delta}{|v_i - v_j|} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ &\leq CR^d \delta^{d-1} + \int \mathbf{1}_{\{|v_i - v_j| > \delta\}} \frac{\delta}{|v_i - v_j|} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \end{aligned}$$

where the first integral was evaluated thanks to (4.70). In the remaining integral, the contribution of the velocities such that  $|v_i - v_j| \geq 1$  can be bounded by  $R^{d+1}\delta$ . Thus it is enough to consider

$$\begin{aligned} & \int \mathbf{1}_{\{1 \geq |v_i - v_j| > \delta\}} \frac{\delta}{|v_i - v_j|} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ &= \delta \int \left( \int_{|v_i - v_j|}^1 \frac{dr}{r^2} + 1 \right) \mathbf{1}_{\{1 \geq |v_i - v_j| > \delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ &\leq \delta \int_{\delta}^1 \frac{dr}{r^2} \int \mathbf{1}_{\{|v_i - v_j| \leq r\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* + CR^{d+1}\delta, \end{aligned}$$

where we used Fubini's Theorem in the last inequality. Applying once again (4.70), we get

$$\int \mathbf{1}_{\{1 \geq |v_i - v_j| > \delta\}} \frac{\delta}{|v_i - v_j|} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^{d+1}\delta \int_{\delta}^1 r^{d-3} dr + CR^{d+1}\delta^{d-1},$$

from which (4.71) follows with a logarithmic singularity if  $d = 2$ .  $\square$

The following lemma provides a counterpart to (4.71) when particle  $j$  is created from particle  $i$ .

**Lemma 4.17.** *Fix a velocity  $\bar{v}_i$  in  $\mathbb{B}_R$  and suppose that  $v_i, v_j$  are given as the velocities after a collision (see Figure 4.5):  $(v_i, v_j) = (\bar{v}_i, v^*)$  or  $(v_i, v_j) = (V', V'_*)$ . Then*

$$\int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \frac{1}{|v_i - v_j|} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^d. \quad (4.72)$$

*Proof.* In both cases, the velocities before and after the collision are related by  $|v_i - v_j| = |v^* - \bar{v}_i|$ . Inequality (4.72) follows from the fact that the singularity  $1/|v^* - \bar{v}_i|$  is integrable.  $\square$

The following result generalizes (4.70) to events such that the relative velocities lie in a given rectangle.

**Lemma 4.18.** *Let  $\mathbf{R}$  be a cylinder of length  $R \gg 1$  and radius  $\delta \leq 1$ . Fix  $\bar{v}_i, v_j$  two velocities in  $\mathbb{B}_R$ . Given the collision parameters  $(v^*, v^*)$ , the velocity  $v_i$  is defined as one of the outgoing velocities  $V'$  or  $V'_*$  in (4.69). We get*

$$\int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \mathbf{1}_{\{v_i - v_j \in \mathbf{R}\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \leq CR^2 \delta^{d-1} (|\log \delta| + \log R). \quad (4.73)$$



*Proof.* In order to deduce Estimate (4.18) from (4.70), the rectangle  $v_j + \mathbf{R}$  is covered by  $\lfloor \frac{R}{\delta} \rfloor$  balls of radius  $2\delta$ . Let  $\omega$  be the axis of the rectangle  $v_j + \mathcal{R}$  and denote by  $w_k = w_0 + \delta k \omega$  the centers of the balls which are indexed by the integer  $k \in \{0, \dots, \lfloor \frac{R}{\delta} \rfloor\}$ . Applying (4.70) to each ball, we get

$$\begin{aligned} & \int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \mathbf{1}_{\{v_i - v_j \in \mathbf{R}\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ & \leq \sum_{k=0}^{\lfloor \frac{R}{\delta} \rfloor} \int_{\mathbb{S}^{d-1} \times \mathbb{B}_R} \mathbf{1}_{\{|v_i - w_k| \leq 2\delta\}} |(v^* - \bar{v}_i) \cdot v^*| dv^* dv^* \\ & \leq CR^d \sum_{k=0}^{\lfloor \frac{R}{\delta} \rfloor} \delta^{d-1} \min\left(\frac{\delta}{|w_k - \bar{v}_i|}, 1\right), \\ & \leq CR^d \delta^{d-1} \sum_{k=0}^{\lfloor \frac{R}{\delta} \rfloor} \frac{\delta}{|w_k - \bar{v}_i| + \delta} \leq CR^d \delta^{d-1} \left(\log\left(\frac{R}{\delta}\right) + 1\right), \end{aligned}$$

where the log divergence in the last inequality occurs from the summation over the coordinates  $w_k$  along the axis of the rectangle. This completes the proof of Lemma 4.18.  $\square$

### 4.3.8 Convergence to the brownian motion

#### Step 1. Finite dimensional marginals.

First, we are going to rewrite the time correlations in terms of collision trees. A similar approach was devised in Lebowitz, Spohn [24] to derive an information on the true particle trajectories (in the physical space) from the Duhamel series.

**Proposition 4.19.** *For any measurable event  $\mathcal{E}$  in  $C([0, T])$*

$$\mathbb{P}_N(\{x_1 \in \mathcal{E}\}) = \int_{\mathbb{T}^d \times \mathbb{R}^d} dz_1 \sum_{m=0}^{N-1} Q_{1,1+m}(T) \mathbf{1}_{\{Y_T \in \mathcal{E}\}} f_{N+1}^{(1+m)}(0),$$

where the series are restricted to the pseudo-trajectories in  $\mathcal{E}$ .

*Proof.* Let  $u_1 < \dots < u_\ell$  be an increasing collection of times and  $H_\ell = \{h_1, \dots, h_\ell\}$  a collection of  $\ell$  smooth functions. Define the biased distribution at time  $t > u_\ell$  as follows

$$\begin{aligned} \int_{\mathbb{T}^{Nd} \times \mathbb{R}^{Nd}} dZ_N f_{N, H_\ell}(t, Z_N) \Phi(Z_N) & := \mathbb{E}_N \left( h_1(x_1(u_1)) \dots h_\ell(x_1(u_\ell)) \Phi(Z_N(t)) \right) \quad (4.74) \\ & = \int_{\mathbb{T}^{Nd} \times \mathbb{R}^{Nd}} dZ_N f_N^0(Z_N) h_1(x_1(u_1)) \dots h_\ell(x_1(u_\ell)) \Phi(Z_N(t)), \end{aligned}$$

for any test function  $\Phi$ .

The corresponding marginals are

$$f_{N, H_\ell}^{(s)}(t, Z_s) := \int f_{N, H_\ell}(t, Z_N) dz_{s+1} \dots dz_N. \quad (4.75)$$

By construction  $f_{N,H_\ell}$  satisfies the Liouville equation for  $t > u_\ell$  and the marginals  $f_{N,H_\ell}^{(s)}$  satisfy the BBGKY hierarchy, introduced in Proposition 3.2. Applying the iterated Duhamel formula in the time interval  $[u_\ell, t]$ , we get

$$f_{N,H_\ell}^{(s)}(t) = \sum_{m=0}^{N-s} \alpha^m Q_{s,s+m}(t - u_\ell) f_{N,H_\ell}^{(s+m)}(u_\ell). \quad (4.76)$$

By construction  $f_{N,H_\ell}(u_\ell, Z_N) = f_{N,H_{\ell-1}}(u_\ell, Z_N) h_\ell(z_1)$ , where the new distribution is now modified by the the first  $\ell - 1$  functions. This procedure can be iterated up to the initial time. The backward dynamics can be understood in terms of collision trees which are now weighted by the factor  $h_1(x_1(u_1)) \dots h_\ell(x_1(u_\ell))$  associated with the motion of the tagged particle

$$f_{N,H_\ell}^{(1)}(t) = \sum_{m_1+\dots+m_\ell=0}^{N-1} Q_{1,1+m_1}(t - u_\ell) \left( h_\ell Q_{1+m_1,1+m_2}(u_\ell - u_{\ell-1}) \left( h_{\ell-1} \dots \right. \right. \\ \left. \left. Q_{1+m_1+\dots+m_{\ell-1},1+m_1+\dots+m_\ell}(u_1) \right) f_N^{(1+m_1+\dots+m_\ell)}(0) \right). \quad (4.77)$$

This identity holds for any  $N$  and any time.

For any  $0 \leq u_1 < \dots < u_\ell \leq T$ , let  $\pi_{u_1, \dots, u_\ell}$  be the projection from  $C([0, T])$  to  $(\mathbb{T}^d \times \mathbb{S}^{d-1})^{\otimes \ell}$

$$\pi_{u_1, \dots, u_\ell}(Y) = (Y(u_1), \dots, Y(u_\ell)). \quad (4.78)$$

The  $\sigma$ -field of Borel sets in  $C([0, T])$  can be generated by the sets of the form  $\pi_{u_1, \dots, u_\ell}^{-1} H$  with  $H \in (\mathbb{T}^d \times \mathbb{S}^{d-1})^\ell$  (see Theorem ?? in [?]). Thus (??) is sufficient to characterize the probability of any measurable set  $\mathcal{E}$ . This completes the proof of Proposition 4.19.  $\square$

### Step 2. The limiting process.

Let  $t_1 < \dots < t_\ell$  be an increasing collection of times and  $H_\ell = \{h_1, \dots, h_\ell\}$  a collection of  $\ell$  smooth functions. As in (4.74), we define  $g_{\alpha, H_\ell}(t)$  as the biased distribution of the Markov chain  $\bar{z}_1(t) = (\bar{x}_1(t), \bar{v}_1(t))$

$$\forall t \in [t_k, t_{k+1}[, \quad \int_{\mathbb{T}^d \times \mathbb{R}^d} g_{\alpha, H_\ell}(t, z) \Phi(z) dz = \mathbb{E}_{M_\beta} \left( h_1(\bar{x}_1(t_1)) \dots h_\ell(\bar{x}_1(t_\ell)) \Phi(\bar{z}_1(t)) \right),$$

with  $t_{\ell+1} = \infty$ . One can consider a measure (cf. (??)) including as well the background density of an ideal gas. The marginals of this measure are

$$g_{\alpha, H_\ell}^{(s)}(t, Z_s) = g_{\alpha, H_\ell}(t, z_1) \prod_{i=2}^s M_\beta(v_i). \quad (4.79)$$

As in (4.77), the distribution can be rewritten in terms of a Duhamel series

$$g_{\alpha, H_\ell}(t) = \sum_{m_1+\dots+m_\ell=0}^{\infty} Q_{1,1+m_1}^0(t - t_\ell) \left( h_\ell Q_{1+m_1,1+m_2}^0(t_\ell - t_{\ell-1}) \left( h_{\ell-1} \dots \right. \right. \\ \left. \left. Q_{1+m_1+\dots+m_{\ell-1},1+m_1+\dots+m_\ell}^0(t_1) \right) g_{\alpha, H_\ell}^{(1+m_1+\dots+m_\ell)}(0) \right). \quad (4.80)$$

This representation allows us to rephrase the Markov chain expectations in terms of the Boltzmann hierarchy. In this series, a lot of cancellations occur (see figure ??). Indeed, the only relevant collision trees are made of a single backbone (the trajectory of  $z_1^0$ ) with branches representing the collisions of  $z_1^0$  with the ideal gas, but no further ramification. In step 3, we shall not use these cancellations and simply compare the series (4.77) and (4.80) term by term in order to show that in the Boltzmann Grad limit when  $\alpha \ll \sqrt{\log \log N}$

$$\lim_{\alpha \rightarrow \infty} \mathbb{E}_{M_\beta} \left( h_1(\bar{x}_1(\alpha\tau_1)) \dots h_\ell(\bar{x}_1(\alpha\tau_\ell)) \right) - \mathbb{E}_N \left( h_1(x_1(\alpha\tau_1)) \dots h_\ell(x_1(\alpha\tau_\ell)) \right) = 0. \quad (4.81)$$

### Step 3. Approximation of the finite dimensional marginals.

We turn now to the proof of (4.81) which combined with (??) will show the convergence (??) of the marginals of the tagged particle sampled at different times.

Suppose now that the collection  $H_\ell$  satisfies the uniform bounds on  $\mathbb{T}^d$

$$\forall i \leq \ell, \quad 0 \leq h_i(x_1) \leq m. \quad (4.82)$$

Thus the  $f_{N,H_\ell}^{(s)}$  satisfy the maximum principle (??) with an extra factor  $m^\ell$ . The pruning procedure on the collision trees therefore applies also in this case and enables us to restrict to trees with at most  $A^{K+1}$  collisions during the time interval  $[0, t]$ . Furthermore, the comparison of the trajectories for  $f_{N,H_\ell}^{(1)}$  and  $g_{\alpha,H_\ell}$  can be achieved in the same way as before on a tree with less than  $A^{K+1}$  collisions and no recollisions. Analogous bounds as in Proposition ?? can be obtained, but one has to take into account that the trees are now weighted by  $h_1(x_1^0(\alpha\tau_1)) \dots h_\ell(x_1^0(\alpha\tau_\ell))$ . We recall that the pseudo-trajectories of  $x_1$  and  $x_1^0$  coincide at any time, thus bounds similar to (4.25) hold

$$\|f_{N,H_\ell}^{(1)}(\alpha\tau, y, v) - g_{\alpha,H_\ell}(\alpha\tau, y, v)\|_{L^\infty(\mathbb{T}^d \times \mathbb{R}^d)} \leq C m^\ell \|\rho^0\|_\infty \left[ \frac{\tau \alpha^2}{(\log \log N)^{\frac{A-1}{A}}} \right]^{\frac{A^2}{A-1}}. \quad (4.83)$$

This implies (4.81), hence (??) thanks to (??).

## 4.4 Related models

### 4.4.1 Lorentz gas

+ weak interactions and quantum Lorentz gas

### 4.4.2 Langevin dynamics

### 4.4.3 The non dilute gas

If the tagged particle velocity evolves according to the Markov process (4.2), then the velocity correlations decay exponentially in time

$$\mathbb{E}_{M_\beta}(v(0)v(t)) \simeq \exp(-ct),$$

this ensures that the diffusion coefficient is finite

$$\mathbf{D} = 2 \int_0^\infty \mathbb{E}_{M_\beta}(v(0) v(t)) dt < \infty. \quad (4.84)$$

For a tagged particle in a hard-sphere gas, the exponential decay is only valid in the Boltzmann-Grad limit and otherwise for low (but non vanishing) densities, it is conjectured that the time correlations decay polynomially

$$\mathbb{E}_{M_\beta}(v(0) v(t)) \simeq \frac{1}{t^{d/2}}.$$

This scaling was discovered numerically in [2] (in  $d = 2, 3$ ) and this comes from the fact that the recollisions are building up correlations. This slow decay leads to an anomalous diffusion in dimension  $d = 2$  as the diffusion coefficient (4.10) diverges.

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