# From molecular dynamics to kinetic theory and hydrodynamics

Thierry Bodineau, Isabelle Gallagher and Laure Saint-Raymond

**Abstract.** In these notes we present the main ingredients of the proof of the convergence of the distribution function of a tagged particle in a background initially at equilibrium, towards the solution to the heat equation. We also show how the process associated with the tagged particle converges in law towards a Brownian motion.

Mathematics Subject Classification (2010). 76P05; 82B21; 82B40

**Keywords.** Boltzmann equation; BBGKY hierarchy; heat equation; Brownian motion ; low density limit ; branching process.

## 1. Introduction

**1.1.** Microscopic and macroscopic models for rarefied gases. At the second International Congress of Mathematicians held in Paris in 1900, D. Hilbert presented ten of his famous list of twenty-three open questions [25]. Some of those questions have since been solved, and some remain open to this day. Among these, we are interested here in the sixth problem related to the axiomatization of physics. The challenge is to understand whether or not the different models describing the dynamics of fluids are consistent, and more precisely to develop "mathematically the limiting processes [...] which lead from the atomistic view to the laws of motion of continua".

**1.1.1. The particle description.** At the atomistic scale, a system of N particles in a domain  $\mathbb{D} \subset \mathbb{R}^d$  can be described by their N positions  $X_N := (x_1, \ldots, x_N)$ in  $\mathbb{D}^N$  and N velocities  $V_N := (v_1, \ldots, v_N)$  in  $\mathbb{R}^{dN}$ , where  $d \geq 2$  denotes the dimension. These evolve according to Newton's laws. For instance assuming that they are identical and interact via a pairwise potential at some scale  $\varepsilon > 0$ , the positions and velocities are related by the following system of ODEs: for  $1 \leq i \leq N$ ,

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

where *m* is the mass of the particles (which we shall assume from now on equal to 1 to simplify) and the force exerted by particle *j* on particle *i* is  $-\frac{1}{\varepsilon} \nabla \Phi\left(\frac{x_i - x_j}{\varepsilon}\right)$ .



Figure 1. The different levels of description of a perfect gas

Note that these equations are nothing else than the Hamiltonian system associated with the energy

$$H_N(X_N, V_N) := \sum_{i=1}^N \frac{1}{2} |v_i|^2 + \sum_{i \neq j} \Phi\left(\frac{x_i - x_j}{\varepsilon}\right).$$

To avoid complicated billiard free dynamics on  $\mathbb{D}$ , we shall focus here on the case of the unit torus  $\mathbb{D} = \mathbb{T}^d := \mathbb{R}^d / \mathbb{Z}^d$ . For the sake of simplicity, we shall further assume that the interaction is pointwise: the particles are N hard spheres of diameter  $\varepsilon > 0$ and centers  $X_N := (x_1, \ldots, x_N)$ , interacting via elastic collisions: namely if there exists  $j \neq i$  such that  $|x_i - x_j| = \varepsilon$ , then the incoming velocities  $(v_i^{in}, v_j^{in})$  are related to the outgoing velocities  $(v_i^{out}, v_j^{out})$  by

where  $\nu^{i,j} := (x_i - x_j)/|x_i - x_j|$ . The wellposedness of this system of ODEs is not an obvious fact, due to the possible clustering of collision times between particles which could lead to a finite-time blow-up, or to the possibility that three or more particles collide at the same time. However it can be proved (see [1, 2] in the case of an infinite number of particles, or [20] for instance in the easier situation under study) that the set of initial configurations leading to such pathologies is of measure zero, hence it will be neglected from now on.

In the following to simplify notation, we shall denote, for  $1 \le i \le N$ ,  $z_i := (x_i, v_i)$ and  $Z_N := (z_1, \ldots, z_N)$ . The distribution function  $f_N(t, Z_N)$  associated with the system (1) satisfies the Liouville equation

$$\partial_t f_N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f_N - \frac{1}{\varepsilon} \sum_{\substack{i=1\\j \neq i}}^N \sum_{\substack{j=1\\j \neq i}}^N \nabla_x \Phi\left(\frac{x_i - x_j}{\varepsilon}\right) \cdot \nabla_{v_i} f_N = 0 \quad \text{in } \mathbb{T}^{dN} \times \mathbb{R}^{dN} \,.$$

In the case of hard-spheres (2) this equation becomes

$$\partial_t f_N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f_N = 0, \qquad (3)$$

and it is set in  $\mathcal{D}_N^{\varepsilon} \times \mathbb{R}^{dN}$  with  $\mathcal{D}_N^{\varepsilon} := \{X_N \in \mathbb{T}^{dN}, \forall i \neq j, |x_i - x_j| > \varepsilon\}$ with a specular reflection on the boundary. We now distinguish pre-collisional configurations from post-collisional ones by defining for indexes  $1 \leq i \neq j \leq N$ 

$$\partial \mathcal{D}_{N,\pm}^{\varepsilon}(i,j) := \left\{ Z_N \in \mathbb{T}^{dN} \times \mathbb{R}^{dN} / |x_i - x_j| = \varepsilon, \quad \pm (v_i - v_j) \cdot (x_i - x_j) > 0 \\ \text{and} \quad \forall (k,\ell) \in \left\{ [1,N] \setminus \{i,j\} \right\}^2, |x_k - x_\ell| > \varepsilon \right\}$$

Given  $Z_N$  on  $\partial \mathcal{D}_{N,+}^{\varepsilon}(i,j)$ , we define  $Z_N^{(i,j)} \in \partial \mathcal{D}_{N,-}^{\varepsilon}(i,j)$  as the configuration having the same positions  $(x_k)_{1 \leq k \leq N}$ , the same velocities  $(v_k)_{k \neq i,j}$  for non interacting particles, and the following pre-collisional velocities for particles i and j

$$v_i^{(i,j)} := v_i - \frac{1}{\varepsilon^2} (v_i - v_j) \cdot (x_i - x_j) (x_i - x_j)$$
  

$$v_j^{(i,j)} := v_j + \frac{1}{\varepsilon^2} (v_i - v_j) \cdot (x_i - x_j) (x_i - x_j).$$
(4)

Then

$$f_N(t, Z_N) = f_N(t, Z_N^{(i,j)})$$
 (5)

with the notation introduced in (4).

J

**1.1.2. From particles to fluids.** From the knowledge of  $Z_N(t)$ , one can define *observable* quantities such as the empirical density, momentum and energy:

$$\rho_N(t,x) := \frac{1}{N} \sum_{i=1}^N \delta\big(x - x_i(t)\big), \quad \rho_N u_N(t,x) = \frac{1}{N} \sum_{i=1}^N v_i(t)\delta\big(x - x_i(t)\big),$$

$$e_N(t,x) := \frac{1}{2} \rho_N(u_N^2 + d\theta_N)(t,x) := \frac{1}{2N} \sum_{i=1}^N |v_i(t)|^2 \delta\big(x - x_i(t)\big).$$
(6)

To obtain laws of motion of continua one starts from those observables and one takes the limit  $N \to \infty$  with  $\varepsilon \to 0$ . By definition, rarefied gases are those for which there is no excluded volume in the state relation, meaning that  $N\varepsilon^d \ll 1$  for the hydrodynamic limit (see Figure 1). Fluid equations are the asymptotic form of the conservations of empirical density, momentum and energy. In order to get a

closed system of equations we need to show that the microscopic fluxes converge to some macroscopic fluxes depending on the macroscopic density  $\rho$ , momentum  $\rho u$ and internal energy e, in the limit  $N \to \infty$ . This convergence has to be understood in the sense of the law of large numbers with respect to the density  $f_N$  (solution to the Liouville equation). The point is therefore to establish that "locally"  $f_N(t)$ is close to an equilibrium measure. This fact is not known in the case of the deterministic dynamics of hard spheres.

By adding a small noise term which exchanges the momenta of nearby particles, Olla, Varadhan and Yau [35] proved the almost sure convergence of the empirical density, velocity and energy to the solution of the Euler equation

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0$$
$$\partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + \rho \theta \mathrm{Id}) = 0$$
$$\partial_t (\rho e) + \nabla_x \cdot (\rho u e + \rho \theta u) = 0$$

as long as it has a smooth solution. The result [35] follows from the ergodicity of the infinite system of interacting particles: the translation invariant stationary measures of the dynamics minimizing the entropy production are the Gibbs measures.

The Navier-Stokes equations are the next order corrections to the Euler equations. In order to derive them one needs to show that the microscopic current is well approximated by the sum of the macroscopic current and a much smaller viscosity term. The mathematical interpretation of this viscous term is given by some fluctuation-dissipation equation. In order to avoid the difficulties of the multiscale asymptotics, we may consider the case when the leading order (compressible) approximation is just a constant and turn to the incompressible Navier-Stokes equations. The rigorous derivation of the incompressible Navier-Stokes equations from particle systems has then been obtained in the framework of stochastic lattice models, first by Esposito, Marra and Yau [19], under some regularity assumption which was later removed by Quastel and Yau [38].

**Remark 1.1.** Note that this approach also provides convergence results for fluids with excluded volume, i.e. when  $N\varepsilon^d = O(1)$ .

**Remark 1.2.** The complexity of the problem is such that there is still no complete derivation of any fluid model starting from the full deterministic Hamiltonian dynamics, regardless of the regime.

**1.1.3. The Boltzmann equation.** In his statement of the sixth problem, Hilbert actually suggested that an intermediate step between the atomistic and the continuous points of view could be the "mesoscopic" scale, governed by the Boltzmann equation obtained in the low density limit  $N \to \infty$ ,  $N\varepsilon^{d-1}\alpha^{-1} = 1$  (see Figure 1). More precisely the idea is to start with the description of the particle system via its distribution function  $f_N$ , satisfying the Liouville equation (3). Then one aims at deriving a closed equation on the probability distribution f(t, x, v) of one particle (describing the probability for a particle to be at time t at position x with

velocity v). As we shall see in the formal derivation in Section 1.2 below, the one-particle density distribution f is the limit (as  $N \to \infty$ ) of

$$f_N^{(1)}(t, z_1) := \int f_N(t, Z_N) \, dz_2 \dots dz_N \,, \tag{7}$$

assuming that  $f_N$  is unchanged under the relabeling of particles, namely

$$f_N(t, Z_{\sigma(N)}) = f_N(t, Z_N), \quad \forall \sigma \in \mathfrak{S}_N.$$

Under the *chaos assumption*, i.e. assuming that the particles are independent and identically distributed, one obtains heuristically that the function f satisfies the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \alpha Q(f, f) \tag{B}$$

with Q, a local operator in x and t, defined by

~

$$Q(f,f) := \int_{\mathbb{S}^{d-1} \times \mathbb{R}^{d-1}} [f(v')f(v_1') - f(v)f(v_1)] b(v - v_1, \omega) \, dv_1 d\omega$$

and  $(v', v'_1)$  are given by  $v' = v + \omega \cdot (v_1 - v) \omega$  and  $v'_1 = v_1 - \omega \cdot (v_1 - v) \omega$ . The function  $b(v - v_1, \omega)$  is the collision kernel. In the case of hard-spheres interacting elastically as in (2), one has

$$b(v - v_1, \omega) = \left(\omega \cdot (v_1 - v)\right)_+.$$

Note that the Boltzmann collision operator Q(f, f) can be split into a gain term and a loss term: the loss term counts all collisions in which a given particle of velocity v will encounter another particle, of velocity  $v_1$ , and thus will change its velocity leading to a loss of particles of velocity v; on the other hand, the gain term measures the number of particles of velocity v which are created due to a collision between particles of velocities v' and  $v'_1$ .

Because particles are indistinguishable, v and  $v_1$  play symmetric roles in the collision integral. The reversibility of the elementary collision process implies moreover that the change of variables  $(v', v'_1, \omega) \rightarrow (v, v_1, \omega)$  has unit jacobian, so that for any smooth function  $\varphi$  defined on  $\mathbb{R}^d$ , one has formally (under suitable decay and smoothness assumptions on f)

$$\int Q(f,f)\varphi(v)dv = \frac{1}{4} \int [f(v')f(v'_1) - f(v)f(v_1)] (\varphi(v) + \varphi(v_1) - \varphi(v') - \varphi(v'_1)) \\ \times ((v-v_1) \cdot \omega)_+ dvdv_1d\omega.$$

In particular, choosing  $\varphi(v) = 1$ , then  $\varphi(v) = v$  and  $\varphi(v) = |v|^2$ , we formally obtain the conservation of mass, momentum and energy

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0, \quad \partial_t (\rho u) + \nabla_x \cdot \int f v \otimes v dv = 0,$$
  
$$\partial_t (\rho u^2 + d\rho \theta) + \nabla_x \cdot \int f |v|^2 v dv = 0,$$

where

$$\begin{aligned} \rho(t,x) &:= \int f(t,x,v) \, dv, \quad \rho u(t,x) := \int f(t,x,v) \, v dv \\ \frac{1}{2} \rho(t,x) \left( |u(t,x)|^2 + d \, \theta(t,x) \right) &= \frac{1}{2} \int f(t,x,v) \, |v|^2 dv \end{aligned}$$

On the other hand, taking  $\varphi = \log f$  in the previous identity, we also get

$$D(f) := -\int Q(f, f) \log f(v) \, dv \ge 0 \,,$$

from which we deduce the entropy inequality, referred to as Boltzmann's H theorem,

$$\int f \log f(t, x, v) dx dv + \alpha \int_0^t \int D(f)(s, x) ds dx \le \int f^0 \log f^0(x, v) dx dv \,,$$

where  $f^0$  is the initial data of f. This means in particular that the Boltzmann equation describes irreversible dynamics. More precisely, we expect the Boltzmann equation to predict a relaxation towards thermodynamic equilibria, which are minimizers of the entropy for fixed mass, momentum and energy. This is in apparent contradiction with the fact that the Liouville equation and Newton's laws are reversible, and satisfy the Poincaré recurrence principle. We shall comment more on that later on (see Remark 1.6).

**Remark 1.3.** Note that, in general, the collision integral does not make sense under the only physical estimates. Formally, the conservations of mass and energy indeed provide

$$\iint f(t, x, v)(1+|v|^2)dvdx = \iint f^0(x, v)(1+|v|^2)dvdx,$$

whereas Boltzmann's H-theorem gives the decay of entropy  $\iint f \log f(t, x, v) dx dv$ . In other words, the collision operator involves the product of two functions of x which are only known to be in some  $L \log L$  Orlicz space.

**1.1.4. From Boltzmann to fluids.** From the works of Hilbert [26] and Chapman-Enskog [12, 16], it is known that most fluid equations can be formally obtained from the Boltzmann equation (B). In the fast relaxation limit  $\alpha \to \infty$ , i.e. when the mean free path  $1/\alpha$  is very small compared to the typical observation length, we indeed expect the collision process to be dominating and the solution to the Boltzmann equation to be close to local thermodynamic equilibrium. The evolution of the gas should therefore be well approximated by fluid equations.

Let us define  $M_f$ , the local Maxwellian of same moments as f, by

$$M_f(t, x, v) := \frac{\rho(t, x)}{(2\pi\theta(t, x))^{\frac{d}{2}}} e^{-\frac{|v-u(t, x)|^2}{2\theta(t, x)}}.$$

At leading order, replacing f by  $M_f$  in the conservation laws, we get the compressible Euler equations. Collecting all contributions to the local thermodynamic

6

equilibrium at leading order, we then introduce the following Ansatz to describe the purely kinetic part of f

$$f = M_f \left( 1 + \sum_{j=1}^{+\infty} \frac{1}{\alpha^j} g_j \right).$$

The crucial point is that the collision operator linearized around  $M_f$ , denoted by  $-\mathcal{L}_{M_f}$ , is a Fredholm operator on  $L^2(M_f dv)$  with kernel spanned by the collision invariants 1, v and  $|v|^2$ . Denoting by  $\Pi^{\perp}$  the projection onto the orthogonal of the kernel of  $-\mathcal{L}_{M_f}$  we get at the next order

$$\mathcal{L}_{M_f} g_1 = -rac{1}{lpha} \Pi^{\perp} \left( rac{v \cdot 
abla_x M_f}{M_f} 
ight) \,.$$

Inverting  $\mathcal{L}_{M_f}$  on the orthogonal of its kernel, one obtains as first correction to the compressible Euler equations the weakly dissipative, compressible Navier-Stokes system with  $O(1/\alpha)$  dissipation terms

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0$$
  
$$\partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + \rho \theta \operatorname{Id}) = \frac{1}{\alpha} \nabla_x \cdot (\kappa_1(\rho, \theta) \nabla_x u)$$
  
$$\partial_t (\rho(|u|^2 + d \theta)) + \nabla_x \cdot (\rho(|u|^2 + (d + 2)\theta)u) = \frac{1}{\alpha} \nabla_x \cdot (\kappa_2(\rho, \theta) \nabla_x \theta)$$
  
$$+ \frac{1}{\alpha} \nabla_x \cdot (\kappa_1(\rho, \theta) \nabla_x u \cdot u)$$

For a more detailed presentation of formal asymptotic expansions, we refer to [39]. Since the solutions of the first order hydrodynamic approximation exhibit singularities such as shocks or discontinuities, the question of their stability after blow-up time seems out of reach at the present time (see [33] before the blow-up time). A natural idea to avoid these complicated questions about the compressible Euler equations is to consider fluctuations around some special solutions, the simplest ones being global equilibria

$$M_{\beta}(v) := \left(\frac{\beta}{2\pi}\right)^{\frac{a}{2}} e^{-\beta|v|^2/2} \,. \tag{8}$$

At present time, this perturbative framework leading to viscous incompressible fluid models is essentially the only one in which unconditional results are available [4, 22, 44], describing the fast relaxation limit. From the formal expansion, we know that the diffusion terms will be of order 1 if time is rescaled by factor  $\alpha$ . We denote by  $\tau = t/\alpha$  the macroscopic time variable. Then, in order for the nonlinear convection term to remain bounded, we need the fluctuation to be at most of order  $\alpha^{-1}$ . This corresponds to having the Mach and Knudsen numbers of the same order of magnitude, which is in agreement with the Von Karman relation for perfect gases giving the Reynolds number as the ratio of the Mach and Knudsen numbers.



Figure 2. Hydrodynamic limits of the Boltzmann equation

**Remark 1.4.** It is important to realize that considering the fast relaxation limit is only possible if the solution f of (B) is known to exist for a time independent of  $\alpha$ . Therefore the mathematical study of hydrodynamic limits requires either additional (regularity and smallness) assumptions on the initial distribution  $f^0$ , or to consider a very weak notion of solution (namely the renormalized solutions introduced by DiPerna and Lions [15]).

1.1.5. From particles to Boltzmann. In order to use the Boltzmann equation as an intermediate step between particles and fluids, the remaining task consists in justifying the limit from  $f_N^{(1)}$  defined in (7) to f, for a large enough time interval so that one can follow with the (known) limit from (B) to fluid equations. The precise setting (in particular the choice of the scaling  $N\varepsilon^{d-1}\alpha^{-1} = 1$  mentioned above) in which to carry out that limit was identified by Grad in [23]. Lanford presented in [29] a detailed scheme of proof, which was completed by a number of authors (see [14, 13, 42] for important contributions in the hard sphere case, and [20, 37] for a complete proof in the hard sphere case as well as the case of a compactly supported, repulsive potential).

However those results only hold for a microscopic time of order  $1/\alpha$ , and therefore it is impossible to this day to carry out sequentially the particle-to-Boltzmann limit followed by the Boltzmann-to-fluid limit. The difficulty is to find a suitable functional framework to prove the propagation of chaos, and more generally to obtain a good control of correlations for long enough times. We indeed do not expect to get better estimates than for the limiting Boltzmann equation (see Remarks 1.3 and 1.4).

In these notes, we show how in a *linear* setting, the full program can go through: the Lanford proof can be made to hold for a long enough time in order to carry out the hydrodynamic limit. The limit equation obtained in our setting is the heat equation: a precise statement is given in Paragraph 1.4 below.

#### 1.2. The Boltzmann-Grad limit for a system of hard spheres.

**1.2.1. The setting.** From now on to simplify we shall restrict our attention to the case of hard-spheres interactions (2), although everything would work in the same way for an adequate, compactly supported repulsive potential (see [20] or [37] for the precise assumptions required on the potential). As explained in Paragraph 1.1.3, the solution to the Boltzmann equation is obtained by taking the limit on the first marginal defined in (7). Let us integrate the Liouville equation (3) over the variables  $(z_2, \ldots, z_N)$ . Using Green's formula to handle the contribution of the boundary, one comes up formally with the following equation on  $f_N^{(1)}$ :

$$\partial_t f_N^{(1)} + v_1 \cdot \nabla_{x_1} f_N^{(1)} = (N-1)\varepsilon^{d-1} \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} f_N^{(2)}(t, x_1, v_1, x_1 + \varepsilon \omega, v_2) \\ \times \left( (v_2 - v_1) \cdot \omega \right) dv_2 d\omega \,,$$

where for  $1 \leq s \leq N$  one denotes

$$f_N^{(s)}(t, Z_s) := \int f_N(t, Z_N) \mathbf{1}_{X_N \in \mathcal{D}_N^{\varepsilon}} dz_{s+1} \dots dz_N$$

The right-hand side can be modified as follows: we split the integral according to

$$\begin{split} \int f_N^{(2)}(t, x_1, x_2 + \varepsilon \omega, v_1, v_2)(v_2 - v_1) \cdot \omega \, dv_2 d\omega \\ &= \int_{(v_2 - v_1) \cdot \omega > 0} f_N^{(2)}(t, x_1, v_1, x_2 + \varepsilon \omega, v_2)(v_2 - v_1) \cdot \omega \, dv_2 d\omega \\ &+ \int_{(v_2 - v_1) \cdot \omega < 0} f_N^{(2)}(t, x_1, v_1, x_2 + \varepsilon \omega, v_2)(v_2 - v_1) \cdot \omega \, dv_2 d\omega \,, \end{split}$$

and in the case when  $(v_2 - v_1) \cdot \omega > 0$  (which corresponds to post-collisional configurations), one can use boundary condition (5) on  $f_N$  to replace the (outgoing) velocities  $(v_1, v_2)$  by (incoming) velocities  $(v'_1, v'_2)$  with according to (2),

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

One then obtains the following equation:

$$\partial_t f_N^{(1)} + v_1 \cdot \nabla_{x_1} f_N^{(1)} = \alpha C_{1,2} f_N^{(2)} \tag{9}$$

with

$$(C_{1,2}f_N^{(2)})(t,x_1,v_1) := (N-1)\varepsilon^{d-1}\alpha^{-1} \int_{\mathbb{S}^{d-1}\times\mathbb{R}^d} \left( f_N^{(2)}(t,x_1,v_1',x_2+\varepsilon\omega,v_2') - f_N^{(2)}(t,x_1,v_1,x_2-\varepsilon\omega,v_2) \right) \left( (v_2-v_1)\cdot\omega \right)_+ dv_2d\omega.$$
(10)

This equation is reminiscent of the Boltzmann equation (B): we recall that taking the limit  $N \to \infty$  we assume that the factor  $(N-1)\varepsilon^{d-1}\alpha^{-1}$  in (10) converges to 1, and moreover if the function  $f_N^{(2)}$  is continuous, then

$$f_N^{(2)}(t, x_1, v_1, x_2 + \varepsilon \omega, v_2) \sim f_N^{(2)}(t, x_1, v_1, x_2, v_2).$$

The main, crucial difference between the equation on  $f_N^{(1)}$  and (B) lies in the fact that there is no reason in general for  $f_N^{(2)}$  to be a product of  $f_N^{(1)}$ . Assuming nevertheless that when N goes to infinity, the following asymptotics hold:

$$f_N^{(1)}(t, z_1) \sim f(t, z_1)$$
 and  $f_N^{(2)}(t, z_1, z_2) \sim f(t, z_1)f(t, z_2)$  (11)

then plugging this Ansatz into (9,10) the function f does satisfy formally the Boltzmann equation (B).

Assumption (11) is wrong for a fixed N because of the interactions between particles. However as N goes to infinity, the chaos property (11) can be shown to hold asymptotically. To make the above argument rigorous, the main difficulty is to prove the propagation of chaos, namely that the almost factorized structure (11) is preserved at time t > 0. Actually the strategy of Lanford consists in proving much more, since the actual hierarchy of equations satisfied by the collection of marginals  $(f_N^{(s)})_{1 \le s \le N}$  is shown to converge, as N goes to infinity under the scaling  $N\varepsilon^{d-1}\alpha^{-1} = 1$ , to a limit (infinite) hierarchy known as the Boltzmann hierarchy. The wellposedness of both hierachies (a prequisite to the convergence) ensures that if the initial data looks like a tensor product, meaning

$$f_{N|t=0}(Z_N) = \frac{1}{\mathcal{Z}_N} \prod_{i=1}^N f^0(z_i) \mathbf{1}_{X_N \in \mathcal{D}_N^\varepsilon}, \quad \mathcal{Z}_N := \int \prod_{i=1}^N f^0(z_i) \mathbf{1}_{X_N \in \mathcal{D}_N^\varepsilon} dZ_N,$$

then so does the solution asymptotically, meaning that as N goes to infinity, in a sense to be made precise one has

$$f_N^{(s)}(t, Z_s) \sim \prod_{i=1}^s f(t, z_i) \mathbf{1}_{X_s \in \mathcal{D}_s^{\varepsilon}}$$

and f must satisfy the Boltzmann equation. In the following to simplify notation we set for  $1 \leq s$ ,

$$f^{\otimes s}(t, Z_s) := \prod_{i=1}^s f(t, z_i) \,.$$

**1.2.2. Statement of the result.** Lanford's theorem may be stated as follows; a sketch of proof is presented in Section 2 (for a complete proof see [20]).

**Theorem 1.5** (From Particles to Boltzmann equation). Let  $d \ge 2$  be given, and consider a nonnegative continuous function  $f^0$  defined on  $\mathbb{T}^d \times \mathbb{R}^d$ . Assume that for some  $\mu_0$  in  $\mathbb{R}$  and  $\beta_0 > 0$ ,

$$f^0(x,v) \le e^{-\mu_0} M_{\beta_0}(v)$$
 and  $\int_{\mathbb{T}^d \times \mathbb{R}^d} f^0(x,v) \, dx \, dv = 1$ .

There exists a time  $T^* > 0$  depending only on  $\mu_0$  and  $\beta_0$  such that the following holds: if  $f_N$  solves (3) with initial data

$$f_{N|t=0}(Z_N) := \mathcal{Z}_N^{-1} (f^0)^{\otimes N} (Z_N) \mathbf{1}_{X_N \in \mathcal{D}_N^{\varepsilon}},$$
  
$$\mathcal{Z}_N := \int (f^0)^{\otimes N} (Z_N) \mathbf{1}_{X_N \in \mathcal{D}_N^{\varepsilon}} dZ_N$$
(12)

then for all  $1 \leq s$ , one has

$$f_N^{(s)}(t, Z_s) \to f^{\otimes s}(t, Z_s) \quad as \quad N \to \infty \quad with \quad N \varepsilon^{d-1} \alpha^{-1} = 1 \,,$$

locally uniformly in  $[0, \alpha^{-1}T^*[\times \Omega_s, where \Omega_s \text{ is given by}]$ 

$$\Omega_s = \{ Z_s \in \mathbb{T}^{sd} \times \mathbb{R}^{sd} \, / \, \forall t \in \mathbb{R}, \forall i \neq j, \quad x_i - x_j - t(v_i - v_j) \neq 0 \}$$

and f solves (B) with initial data  $f^0$ .

In particular the first marginal does converge, almost everywhere, to the solution of the Boltzmann equation (B).

**Remark 1.6.** The limiting process entails a loss of information which causes irreversibility: the exact position of the particles is indeed lost, and the deflection angle becomes a random parameter.

In the case when the particles are not initially independent, the convergence still holds as proved in [20], but the asymptotics is generally not described by a closed equation on the first marginal. Under suitable assumptions (bounds and convergence) on the initial marginals  $(f_{N|t=0}^{(s)})_{1\leq s\leq N}$ , the limiting marginals  $(f^{(s)})_{s\geq 1}$  satisfy an infinite hierarchy of equations, referred to as Boltzmann's hierarchy. Particular solutions of this hierarchy are

- the chaotic solutions already mentioned  $f^{(s)} = f^{\otimes s}$  with f solution to the full nonlinear Boltzmann equation (B);
- fluctuations describing the dynamics of a tagged particle in a background at equilibrium

$$f^{(s)}(t, Z_s) = M_{\beta}^{\otimes s}(V_s)\varphi_{\alpha}(t, z_1)$$

where  $\varphi_{\alpha}$  is a solution to the *linear Boltzmann equation*:

$$\partial_t \varphi_\alpha + v \cdot \nabla_x \varphi_\alpha = -\alpha L(\varphi_\alpha) \tag{LB}$$

with

$$L(\varphi_{\alpha}) := \iint [\varphi_{\alpha}(v) - \varphi_{\alpha}(v')] M_{\beta}(v_1) b(v - v_1, \omega) dv_1 d\omega.$$

Note that in both cases the closure of the hierarchy is encoded in the particular form of the initial data.

1.3. From the linear Boltzmann equation to the heat equation. As noticed above, it is difficult to go from particles to fluids via the Boltzmann equation, because Lanford's theorem is only true for times which are a priori not uniformly bounded from below with  $\alpha$  (see Theorem 1.5 above). However in the linear setting (LB), global solutions for the limit equation exists. It has been known for a long time that the hydrodynamic limit of (LB) is the heat equation. As stated in [24, 26], L is a Fredholm operator of domain  $L^2(\mathbb{R}^d, aM_\beta dv)$  with

$$a(v) := \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} M_\beta(v_1) \left( (v - v_1) \cdot \omega \right)_+ d\omega dv_1 \, d$$

and its kernel reduces to the constant functions. We can then define the vector  $b(v) = (b_k(v))_{k \le d} \in (\text{Ker } L)^{\perp}$  by  $Lb_k(v) = v_k$  for all  $k \le d$ , and the diffusion coefficient

$$\kappa_{\beta} := \int_{\mathbb{R}^d} v \cdot b(v) \ M_{\beta}(v) dv \,. \tag{13}$$

The following result holds (see for instance [3, 36]).

**Theorem 1.7** (From Linear Boltzmann to the heat equation). Let  $\rho^0$  be a function in  $C^4(\mathbb{T}^d)$  and let  $\rho$  be the unique, bounded solution to

$$\partial_{\tau}\rho - \kappa_{\beta}\Delta_{x}\rho = 0 \quad in \quad \mathbb{T}^{d} \,, \quad \rho_{|\tau=0} = \rho^{0} \,. \tag{14}$$

Let  $\varphi_{\alpha}$  be the unique solution to (LB) with initial data  $\varphi_{\alpha|t=0} = \rho^0$ . Then for all T > 0 there is a constant  $C_T > 0$  such that

$$\sup_{\in [0,T]} \sup_{(x,v)\in\mathbb{T}^d\times\mathbb{R}^d} \left| \left(\varphi_{\alpha}(\alpha\tau, x, v) - \rho(\tau, x)\right) M_{\beta}(v) \right| \le C_T \alpha^{-1}$$

**Remark 1.8.** The same result holds in the more general case when the initial data  $\varphi_{\alpha|t=0}$  to (LB) depends on both variables x and v. In the whole of this text we choose to simplify the presentation by considering only the well-prepared case when  $\varphi_{\alpha|t=0}(x, v) = \rho^0(x)$ , although the proofs to follow may be adapted to a more general situation  $\varphi_{\alpha|t=0} = \varphi^0(x, v)$ .

**1.4.** Statement of the result. In these notes we present a convergence result from an interacting particle system to the heat equation (and the Brownian motion), using the linear Boltzmann equation as an intermediate step. As mentioned in Paragraph 1.2.2, the linear Boltzmann equation can be understood as the limit of the one-particle distribution corresponding to one (or a few) tagged particle in a background of particles initially at equilibrium. The heat equation should therefore be the equation satisfied by the limit of that one-particle distribution, after an adequate rescaling of the time and the density of the background particles. The result proved in [6] is the following.

**Theorem 1.9** (From particles to the heat equation). Consider N hard spheres on the space  $\mathbb{T}^d \times \mathbb{R}^d$ , initially distributed according to the distribution

$$f_N^0(Z_N) := \mathcal{Z}_N^{-1} \mathbf{1}_{\mathcal{D}_{\varepsilon}^N}(X_N) \rho^0(x_1) M_{\beta}^{\otimes N}(V_N) ,$$
  
with  $\mathcal{Z}_N := \int \mathbf{1}_{\mathcal{D}_{\varepsilon}^N}(X_N) dX_N ,$  (15)

where  $\rho^0 \leq C_0$  is a continuous, of integral one, function on  $\mathbb{T}^d$ . Then the distribution  $f_N^{(1)}(\alpha\tau, x, v)$  remains close for the  $L^{\infty}$ -norm to the solution  $\rho(\tau, x)M_{\beta}(v)$  of the linear heat equation (14):

$$\sup_{\tau \in [0,T]} \sup_{(x,v) \in \mathbb{T}^d \times \mathbb{R}^d} \left| f_N^{(1)}(\alpha \tau, x, v) - \rho(\tau, x) M_\beta(v) \right| \to 0$$

in the limit  $N \to \infty$ , with  $\alpha$  going to infinity much slower than  $\sqrt{\log \log N}$ , and with  $N\varepsilon^{d-1}\alpha^{-1} = 1$ . In the same asymptotic regime, the process  $\Xi(\tau) = x_1(\alpha\tau)$ associated with the tagged particle converges in law towards a Brownian motion of variance  $\kappa_{\beta}$ , initially distributed under measure  $\rho^0$ .

The long time behavior of a particle in a medium (Lorentz gas, weak interactions...) has been widely studied and we refer to [41] for a survey of the models and results.

In the framework described in this paper, the convergence of  $f_N^{(1)}(t, x, v)$  to the solution of the linear Boltzmann equation has been shown to hold in the Boltzmann-Grad limit for any time t > 0 in [5, 30]. The convergence in Theorem 1.9 however is quantitative and therefore allows us to obtain controls of the distribution for times  $t = \alpha \tau$  diverging with N.

The case of a Lorentz gas is somewhat different in nature, since the tagged particle moves in a frozen background (see [32] for a survey). Many results have been obtained in that direction : see for instance [21, 8] for the convergence of the distribution of the tagged particle to the solution of (LB) and [11] for the convergence to the brownian motion. In the quantum counterpart of the Lorentz gas, the convergence to the quantum Brownian motion has been derived in [18, 17] and these approaches use a truncation of series which is reminiscent of the method explained in Section 3.3 (see also [31]).

### 2. Proof of Lanford's theorem

In this section we shall give the main steps of the proof of Theorem 1.5. We refer to [20] for all the details.

**2.1. The BBGKY hierarchy.** We recall that the equation satisfied by the first marginal  $f_N^{(1)}$  given in (9) involves the second marginal  $f_N^{(2)}$ . In order to analyze this equation, it is therefore necessary to write the equation satisfied by  $f_N^{(2)}$ , which involves  $f_N^{(3)}$ ..., and so we are finally naturally led to studying the full hierarchy of equations given formally by

$$\partial_t f_N^{(s)} + V_s \cdot \nabla_{X_s} f_N^{(s)} = \alpha C_{s,s+1} f_N^{(s+1)}$$
(16)

with

$$C_{s,s+1}f_N^{(s+1)}(t, Z_s) := (N-s)\varepsilon^{d-1}\alpha^{-1}\sum_{i=1}^s \int_{\mathbb{S}^{d-1}\times\mathbb{R}^d} \omega \cdot (v_{s+1} - v_i) \times f_N^{(s+1)}(t, Z_s, x_i + \varepsilon\omega, v_{s+1})d\omega dv_{s+1}.$$
(17)

This operator can be split into a gain and a loss term, depending on the sign of  $\omega \cdot (v_{s+1} - v_i)$ : we write  $C_{s,s+1} = C_{s,s+1}^+ - C_{s,s+1}^-$ , where

$$C_{s,s+1}^{\pm} f_N^{(s+1)} = \sum_{i=1}^s C_{s,s+1}^{\pm,i} f_N^{(s+1)}$$
(18)

the index i referring to the index of the interaction particle among the s "fixed" particles, with the notation

$$(C_{s,s+1}^{\pm,i} f_N^{(s+1)})(Z_s) := (N-s)\varepsilon^{d-1}\alpha^{-1} \int_{\mathbb{S}^{d-1} \times \mathbb{R}^d} (\omega \cdot (v_{s+1} - v_i))_{\pm} \\ \times f_N^{(s+1)}(Z_s, x_i + \varepsilon \omega, v_{s+1}) \, d\omega \, dv_{s+1} \,,$$
(19)

the index + corresponding to post-collisional configurations and the index - to pre-collisional configurations. This hierarchy of equations is known as the BBGKY hierarchy, after N. Bogoliubov [7], M. Born, and H. S. Green [9], J. G. Kirkwood [27] and J. Yvon [45].

**2.2. The Boltzmann hierarchy.** From the BBGKY hierarchy presented in the previous paragraph, we can formally derive the limiting hierarchy, referred to as Boltzmann's hierarchy. Consider a set of particles  $Z_{s+1} = (Z_s, x_i + \varepsilon \omega, v_{s+1})$ such that  $(x_i, v_i)$  and  $(x_i + \varepsilon \omega, v_{s+1})$  are post-collisional:  $(x_{s+1} - x_i) \cdot (v_{s+1} - v_i) > 0$ . We recall the boundary condition (5)

$$f_N^{(s+1)}(t, Z_s, x_i + \varepsilon \omega, v_{s+1}) = f_N^{(s+1)}(t, Z_s^*, x_i + \varepsilon \omega, v_{s+1}^*)$$

where  $Z_s^* = (z_1, \ldots, z_i^*, \ldots z_s), x_i^* := x_i$  and  $(v_i^*, v_{s+1}^*)$  are the pre-collisional velocities:

$$v_i^* := v_i - \omega \cdot (v_i - v_{s+1}) \omega$$
,  $v_{s+1}^* := v_{s+1} + \omega \cdot (v_i - v_{s+1}) \omega$ .

Then neglecting the spatial micro-translations in the arguments of  $f_N^{(s+1)}$  we formally obtain from (19) the following asymptotic expression for the collision operator at the limit:

$$C_{s,s+1}^0 = C_{s,s+1}^{0+} - C_{s,s+1}^{0-},$$

with

$$C_{s,s+1}^{0+} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ \\ \times f^{(s+1)}(t, x_1, v_1, \dots, x_i, v_i^*, \dots, x_s, v_s, x_i, v_{s+1}^*) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s, x_i, v_{s+1}) d\omega dv_{s+1} + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) := \sum_{i=1}^{s} \int \left( \omega \cdot (v_{s+1} - v_i) \right)_+ f^{(s+1)}(t, Z_s) + \\ C_{s,s+1}^{0-} f^{(s+1)}(t, Z_s) + \\ C_{s,s+1$$

At this stage, the Boltzmann hierarchy is introduced as the formal limit of the BBGKY hierarchy and the core of Lanford's strategy is to justify the convergence. Note also that the Boltzmann hierarchy involves an infinite number of recursive equations for the functions  $\{f^{(s)}\}_{s\geq 1}$ , as opposed to the BBGKY hierarchy which couples only the density marginals up to N.

From molecular dynamics to kinetic theory and hydrodynamics

**2.3. The iterated Duhamel formula.** In order to prove the convergence of  $f_N^{(s+1)}$  to  $f^{(s+1)}$  for a fixed *s* let us write the solutions  $f_N^{(s+1)}$  and  $f^{(s+1)}$  by Duhamel's formula. Denoting by  $\Psi_s(t)$  the *s*-particle flow associated with the hard-sphere system, and by  $\mathbf{T}_s$  the associated solution operator, we have formally

$$f_N^{(s)}(t) = \mathbf{T}_s(t) f_{N|t=0}^{(s)} + \int_0^t \mathbf{T}_s(t-\tau) C_{s,s+1} f_N^{(s+1)}(\tau) \, d\tau \, .$$

Since we distinguish between pre-collisional and post-collisional configurations, we expect the initial data to play a special role. We therefore iterate the previous Duhamel formula to express the solution to the BBGKY hierarchy as an operator acting on the initial data :

$$f_N^{(s)}(t) = \sum_{k=0}^{N-s} \alpha^k \int_0^t \int_0^{t_1} \dots \int_0^{t_{k-1}} \mathbf{T}_s(t-t_1) C_{s,s+1} \mathbf{T}_{s+1}(t_1-t_2) \dots$$

$$\dots \mathbf{T}_{s+k}(t_k) f_{N|t=0}^{(s+k)} dt_k \dots dt_1 .$$
(20)

Similarly the solution to the Boltzmann hierarchy can be recast as

$$f^{(s)}(t) = \sum_{k=0}^{\infty} \alpha^k \int_0^t \int_0^{t_1} \dots \int_0^{t_{k-1}} \mathbf{S}_s(t-t_1) C_{s,s+1}^0 \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2}^0 \dots \dots \mathbf{S}_{s+k}(t_k) f_{|t=0}^{(s+k)} dt_k \dots dt_1,$$
(21)

where  $\mathbf{S}_{s}(t)$  denotes the *s*-particle free-flow.

The goal is now to prove the convergence from (20) to (21) as N goes to infinity with  $N\varepsilon^{d-1}\alpha^{-1} = 1$  and  $1 \leq s$  is fixed. Several points need to be adressed:

- 1. the convergence of both series (20) and (21) over k (uniformly in N);
- 2. the convergence of the initial data  $f_{N|t=0}^{(s+k)}(Z_{s+k})$  to  $f_{|t=0}^{(s+k)}(Z_{s+k})$ ;
- 3. the convergence of the collision operators  $C_{s,s+1}$  to  $C_{s,s+1}^0$ ;
- 4. the convergence of the transport operators  $\mathbf{T}_s$  to  $\mathbf{S}_s$ .

Point 2 is not totally obvious due to the singularities induced by the conditioning associated to the exclusion in  $f_{N|t=0}^{(s+k)}$ . However, defining

$$\mathcal{Z}_N := \int_{\mathbb{R}^{2dN}} \mathbf{1}_{X_N \in \mathcal{D}_N^{\varepsilon}} (f^0)^{\otimes N}(Z_N) \, dZ_N \,,$$

standard arguments lead to

$$1 \leq \mathcal{Z}_N^{-1} \mathcal{Z}_{N-s} \leq \left( 1 - C\varepsilon \| f^0 \|_{L^{\infty}(\mathbb{R}^d_x, L^1(\mathbb{R}^d_v))} \right)^{-s},$$
(22)

and this estimate leads to the expected convergence outside the diagonals.

Point 3 was formally studied in the Paragraph 2.2 and we shall not detail this argument further. Note that the continuity along the normal vector to the boundary (and hence the definition of the trace at the boundary) is obtained recursively by construction of the elementary terms of the series as combinations of collision and transport operators applied to the initial data. Continuity of the initial data  $f^0$  is required in order to prove that the effects of the spatial micro-translations in the collisions will be negligible. In the next two paragraphs we shall concentrate on the more difficult points 1. (Paragraph 2.4) and 4. (Paragraph 2.5).

**2.4. Uniform bounds.** In order to obtain uniform a priori bounds for solutions to the BBGKY and Boltzmann hierarchies, we need to introduce some norms on the space of sequences  $(g^{(s)})_{s\geq 1}$ . These norms, although not exactly equivalent, are inspired from the ensemble formalism in statistical physics. At the canonical level, given  $\varepsilon > 0$ ,  $\beta > 0$ , an integer  $s \geq 1$ , and a measurable function  $g_s: \mathcal{D}_s^{\varepsilon} \times \mathbb{R}^{ds} \to \mathbb{R}$ , we let

$$|g_s|_{\varepsilon,s,\beta} := \operatorname{supess}_{Z_s \in \mathcal{D}_s^{\varepsilon} \times \mathbb{R}^{ds}} \left( |g_s(Z_s)| \exp\left(\frac{\beta}{2} |V_s|^2\right) \right) \,. \tag{23}$$

We also define, for a continuous function  $g_s : \mathbb{T}^{ds} \times \mathbb{R}^{ds} \to \mathbb{R}$ ,

$$|g_s|_{0,s,\beta} := \sup_{Z_s \in \mathbb{T}^{d_s} \times \mathbb{R}^{d_s}} \left( |g_s(Z_s)| \exp\left(\frac{\beta}{2} |V_s|^2\right) \right) \,.$$

Next we denote by  $X_{\varepsilon,s,\beta}$  the Banach space of measurable functions from  $\mathcal{D}_s^{\varepsilon} \times \mathbb{R}^{ds}$  to  $\mathbb{R}$  with finite  $|\cdot|_{\varepsilon,s,\beta}$  norm, and similarly  $X_{0,s,\beta}$  denotes the Banach space of continuous functions from  $\mathbb{T}^{ds} \times \mathbb{R}^{ds}$  to  $\mathbb{R}$  with finite  $|\cdot|_{0,s,\beta}$  norm. At the grand-canonical level, for sequences of functions  $G = (g_s)_{s\geq 1}$ , with  $g_s : \mathcal{D}_s^{\varepsilon} \times \mathbb{R}^{ds} \to \mathbb{R}$ , we let for  $\varepsilon > 0, \beta > 0$ , and  $\mu \in \mathbb{R}$ ,

$$\|G\|_{\varepsilon,\beta,\mu} := \sup_{s \ge 1} \left( |g_s|_{\varepsilon,s,\beta} \exp(\mu s) \right)$$

We define similarly for  $G = (g_s)_{s>1}$ , with  $g_s : \mathbb{T}^{ds} \times \mathbb{R}^{ds} \to \mathbb{R}$  continuous,

$$||G||_{0,\beta,\mu} := \sup_{s \ge 1} \left( |g_s|_{0,s,\beta} \exp(\mu s) \right).$$

Finally we denote  $\mathbf{X}_{\varepsilon,\beta,\mu}$  the Banach space of sequences of functions  $G = (g_s)_{s\geq 1}$ , with  $g_s \in X_{\varepsilon,s,\beta}$  and  $\|G\|_{\varepsilon,\beta,\mu} < \infty$  and similarly  $\mathbf{X}_{0,\beta,\mu}$  is the Banach space of sequences of continuous functions  $G = (g_s)_{s\geq 1}$ , with  $g_s \in X_{0,s,\beta}$  and  $\|G\|_{0,\beta,\mu} < \infty$ . The conservation of energy for the *s*-particle flow is reflected in identities

$$|\mathbf{T}_s(t)g_s|_{\varepsilon,s,\beta} = |g_s|_{\varepsilon,s,\beta}$$
 and  $|\mathbf{S}_s(t)h_s|_{0,s,\beta} = |h_s|_{0,s,\beta}$ 

for all parameters  $\beta > 0$ ,  $\mu \in \mathbb{R}$ , and for all  $g_s \in X_{\varepsilon,s,\beta}$  and  $h_s \in X_{0,s,\beta}$ . The collision operators  $C_{s,s+1}$  and  $C_{s,s+1}^0$  on the other hand involve a linear loss in s and in the velocity variable, since one can check that for almost every t > 0, and almost everywhere in  $Z_s$ ,

$$\left| \left( \mathbf{T}_{s}(-t)C_{s,s+1}\mathbf{T}_{s+1}(t)g_{s+1} \right)(Z_{s}) \right| \\ \leq C \,\beta^{-\frac{d}{2}} \left( s\beta^{-\frac{1}{2}} + \sum_{1 \leq i \leq s} |v_{i}| \right) e^{-\frac{\beta}{2}|V_{s}|^{2}} |g_{s+1}|_{\varepsilon,s+1,\beta} \,, \tag{24}$$

and

$$\left(C_{s,s+1}^{0}g_{s+1}\right)(Z_{s})\right| \leq C \,\beta^{-\frac{d}{2}} \left(s\beta^{-\frac{1}{2}} + \sum_{1 \leq i \leq s} |v_{i}|\right) e^{-\frac{\beta}{2}|V_{s}|^{2}} |g_{s+1}|_{0,s+1,\beta} \,. \tag{25}$$

As pointed out above, in order to make sense of the trace at the boundary it is necessary to study  $\mathbf{T}_{s}(-t)C_{s,s+1}\mathbf{T}_{s+1}(t)$  and not the operator  $C_{s,s+1}$  alone (see [40] for a detailed discussion). The idea behind analytical type results is to compensate the loss of continuity in (24) and (25) (giving rise typically to a factor s(s + 1) $1 \cdots (s+k-1)$  in the elementary terms of the Duhamel expansions (20) and (21) by the successive time integrations (leading to a factor  $t^k/k!$ ). We then expect the series in k to be convergent for small values of  $\alpha t$ . More precisely, it follows from rather standard arguments of the Cauchy-Kowalewski type (see [34] or [43]) that for an initial data bounded in  $\mathbf{X}_{\varepsilon,\beta_0,\mu_0}$  then the solution to the BBGKY hierarchy at time t is bounded in  $\mathbf{X}_{\varepsilon,\beta_0-c\alpha t,\mu_0-c\alpha t}$  for some fixed c > 0, as long as  $\beta_0 - c\alpha t > 0$ . A similar result holds for the Boltzmann hierarchy: if the initial data is bounded in  $\mathbf{X}_{0,\beta,\mu}$  then the solution to the Boltzmann hierarchy at time t is bounded in  $\mathbf{X}_{0,\beta_0-c\alpha t,\mu_0-c\alpha t}$ , as long as  $\beta_0-c\alpha t>0$ . This explains why the Lanford theorem only holds for a short time in general: it is the time for which one can guarantee a uniform bound for all the terms in the hierarchy. We shall call  $[0, T^*/\alpha]$  this life span from now on (where  $T^*$  depends only on  $\beta_0$  and  $\mu_0$ ).

**Remark 2.1.** Actually the precise estimates of [20] show that  $T^*$  is essentially proportional to  $\exp(\mu_0)$ , which controls the weighted norm  $|f^0|_{0,1,\beta}$ . This corresponds typically to the life span we would obtain for the quadratic Boltzmann equation (B) developing a simple  $L^{\infty}$  theory.

**2.5. Termwise convergence.** From now on we fix  $T^*$  as obtained in the previous section and we consider a time  $t \leq T/\alpha$  with  $T < T^*$ . We shall prove the termwise convergence of each marginal to the solution of the limit hierarchy. **2.5.1. Series truncation, cut-off of high energies and of clustering collision times.** The bounds obtained in the previous paragraph imply by the dominated convergence theorem that it is enough to consider finite sums of elementary functions

$$f_{N,R,\delta}^{(s,k)}(t) := \alpha^k \int_{\mathcal{T}_{k,\delta}(t)} \mathbf{T}_s(t-t_1) C_{s,s+1} \mathbf{T}_{s+1}(t_1-t_2) C_{s+1,s+2} \dots \\ \dots \mathbf{T}_{s+k}(t_k) \mathbf{1}_{|V_{s+k}| \le R} f_{N|t=0}^{(s+k)} \, dT_k \,,$$
$$f_{R,\delta}^{(s,k)}(t) := \alpha^k \int_{\mathcal{T}_{k,\delta}(t)} \mathbf{S}_s(t-t_1) C_{s,s+1}^0 \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2}^0 \dots \\ \dots \mathbf{S}_{s+k}(t_k) \mathbf{1}_{|V_{s+k}| \le R} f_{|t=0}^{(s+k)} \, dT_k \,.$$

where  $\mathbb{R}^2$  is a cut-off on the high energies and we have defined

$$\mathcal{T}_{k}(t) := \left\{ T_{k} = (t_{1}, \dots, t_{k}) / t_{i} < t_{i-1} \text{ with } t_{k+1} = 0 \text{ and } t_{0} = t \right\},$$
$$\mathcal{T}_{k,\delta}(t) := \left\{ T_{k} \in \mathcal{T}_{k}(t) / t_{i} - t_{i+1} \ge \delta \right\}.$$

Indeed defining

$$f_N^{(s,k)}(t) := \alpha^k \int_0^t \int_0^{t_1} \dots \int_0^{t_{k-1}} \mathbf{T}_s(t-t_1) C_{s,s+1} \mathbf{T}_{s+1}(t_1-t_2) C_{s+1,s+2} \dots \\ \dots \mathbf{T}_{s+k}(t_k) f_{N|t=0}^{(s+k)} dt_k \dots dt_1$$
$$f^{(s,k)}(t) := \alpha^k \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s(t-t_1) C_{s,s+1}^0 \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2}^0 \dots \\ \dots \mathbf{S}_{s+k}(t_k) f_{|t=0}^{(s+k)} dt_k \dots dt_1,$$

one can check that for each given  $s \ge 1$  and  $t \in [0, T/\alpha]$  there is a constant  $C_s > 0$  depending only on  $\beta_0$ ,  $\mu_0$  and s such that for each  $n \ge 1$ ,

$$\begin{split} \left\| f_{N}^{(s)}(t) - \sum_{k=0}^{n} f_{N}^{(s,k)}(t) \right\|_{L^{\infty}(\mathcal{D}_{s}^{\varepsilon} \times \mathbb{R}^{d_{s}})} + \left\| f^{(s)}(t) - \sum_{k=0}^{n} f^{(s,k)}(t) \right\|_{L^{\infty}(\mathbb{T}^{d_{s}} \times \mathbb{R}^{d_{s}})} \\ + \left\| \sum_{k=0}^{n} (f_{N}^{(s,k)} - f_{N,R,\delta}^{(s,k)})(t) \right\|_{L^{\infty}(\mathcal{D}_{s}^{\varepsilon} \times \mathbb{R}^{d_{s}})} + \left\| \sum_{k=0}^{n} (f^{(s,k)} - f^{(s,k)}_{R,\delta})(t) \right\|_{L^{\infty}(\mathbb{T}^{d_{s}} \times \mathbb{R}^{d_{s}})} \\ & \leq C_{s} \left( \frac{1}{2} \right)^{n} + Ce^{-C'\beta_{0}R^{2}} + Cn^{2} \frac{\delta\alpha}{T} \end{split}$$

uniformly in N and  $t \leq T/\alpha$ , in the Boltzmann-Grad scaling  $N\varepsilon^{d-1}\alpha^{-1} = 1$ . Theorem 1.5 will therefore follow from the convergence of the elementary functions.

**2.5.2. Straightening of trajectories.** The main step of the proof now consists in decomposing the previous truncated functions according to the history of collisions: we write

$$f_{N,R,\delta}^{(s,k)}(t) = \sum_{J,S} \Big(\prod_{i=1}^{k} j_i\Big) f_{N,R,\delta}^{(s,k)}(t,J,S) \quad \text{and} \quad f_{R,\delta}^{(s,k)}(t) = \sum_{J,S} \Big(\prod_{i=1}^{k} j_i\Big) f_{R,\delta}^{(s,k)}(t,J,S)$$

18

with

$$f_{N,R,\delta}^{(s,k)}(t,J,S) := \alpha^k \int_{\mathcal{T}_{k,\delta}(t)} \mathbf{T}_s(t-t_1) C_{s,s+1}^{j_1,\sigma_1} \mathbf{T}_{s+1}(t_1-t_2) C_{s+1,s+2}^{j_2,\sigma_2} \\ \dots \mathbf{T}_{s+k}(t_k-t_{k+1}) \mathbf{1}_{|V_{s+k}| \le R} f_{N|t=0}^{(s+k)} dT_k ,$$
  
$$f_{R,\delta}^{(s,k)}(t,J,S) := \alpha^k \int_{\mathcal{T}_{k,\delta}(t)} \mathbf{S}_s(t-t_1) C_{s,s+1}^{0,j_1,\sigma_1} \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2}^{0,j_2,\sigma_2} \\ \dots \mathbf{S}_{s+k}(t_k-t_{k+1}) \mathbf{1}_{|V_{s+k}| \le R} f_{|t=0}^{(s+k)} dT_k ,$$

where  $J := (j_1, \ldots, j_k) \in \{+, -\}^k$  and the  $\pm$  signs were introduced in (18) to distinguish incoming from outgoing collisions, while  $S := (\sigma_1, \ldots, \sigma_k)$  with  $\sigma_i$ in  $\{1, \ldots, s + i - 1\}$  is the label of the particle colliding with particle s + i. Each one of the functionals  $f_{N,R,\delta}^{(s,k)}(t,J,S)$  and  $f_{R,\delta}^{(s,k)}(t,J,S)$  can be viewed as the contribution associated with some dynamics, which of course is not the actual dynamics in physical space: the characteristics associated with the operators  $\mathbf{T}_{s+i}(t_i - t_{i+1})$  and  $\mathbf{S}_{s+i}(t_i - t_{i+1})$  are followed backwards in time between two consecutive times  $t_i$  and  $t_{i+1}$ , and collision terms (associated with  $C_{s+i,s+i+1}^{j_i,\sigma_i}$ and  $C_{s+i,s+i+1}^{0,j_i,\sigma_i}$ ) are seen as source terms, in which, in the words of Lanford [29], "additional particles" are "adjoined" to the marginal. These dynamics are therefore referred to as "pseudo-trajectories".

The end of the proof of Theorem 1.5 consists in straightening out the BBGKY pseudo-trajectories, for them to become asymptotically close to the Boltzmann pseudo-trajectories (which are straight lines between each collision time  $t_i$  and  $t_{i+1}$ ). This is the most technical part of the proof, as between two collision times  $t_i$ and  $t_{i+1}$ , the BBGKY pseudo-trajectories are not always straight lines since recollisions may occur. These recollisions are eliminated recursively: when a new particle s + i is adjoined at time  $t_i$ , given the other particles (numbered from 1) to s + i - 1, it is possible to choose the velocity and impact parameter of that new particle s + i in a set of almost full measure as N goes to infinity so that after collision or scattering with particle (this depends on whether the particle is incoming or outgoing), the set of s+i particles will stay at a prescribed distance  $\varepsilon_0$ one from another for all times  $t \leq t_i - \delta$ . The main point here is that this geometric argument needs to be applied only a finite number of times since the series has been truncated. It is also important at this stage that velocities are not too big, and that collision times do not cluster. The previous preparation steps are therefore crucial here.

We shall not present the details of the construction, which is rather long and technical, but to give a flavor of the argument let us state one typical geometric result which plays an important role in the proof. In the following we denote by dist the distance on the torus.

**Lemma 2.2.** Let  $x_1, x_2 \in \mathbb{T}^d$  be given such that  $\operatorname{dist}(x_1, x_2) \geq \varepsilon_0 \gg \varepsilon$ , and a velocity  $v_1$  such that  $|v_1| \leq R < \infty$ . Given  $\delta, t > 0$ , there is a set  $K(x_1 - x_2)$  of

small measure:

$$|K(x_1 - x_2)| \le CR^d \left( \left(\frac{\varepsilon}{\varepsilon_0}\right)^{d-1} + \left(\frac{\varepsilon_0}{R\delta}\right)^{d-1} + (Rt)^d \varepsilon_0^{d-1} \right)$$

such that for any velocity  $v_2 \notin (v_1 + K(x_1 - x_2))$ , with  $|v_2| \leq R$ , then

- (i) there is no collision over [0,t] by the backward flow: for any  $\tau \in [0,t]$ , one has dist $(x_1 v_1\tau, x_2 v_2\tau) > \varepsilon$ ;
- (ii) the particles are well separated after a time  $\delta$ : for all times  $\tau \in [\delta, t]$ , there holds dist $(x_1 v_1\tau, x_2 v_2\tau) > \varepsilon_0$ .

The parameter  $\varepsilon_0$  ensures that the pseudo-trajectories are separated and therefore do not recollide. Result (ii) is the main point enabling one to proceed with an inductive proof : with large probability, the pseudo-trajectories in both hierarchies can be coupled and will remain very close to each other up to time 0. At time 0, the cloud of particles will have positions almost identical in both hierarchies up to small shifts of order  $n\varepsilon$ . As the initial densities  $f_{N|t=0}^{(n)}$  and  $f_{|t=0}^{(n)}$  are very close in the large N limit, the small shift of the particles can be bounded by using the gradient norm  $\|\nabla_x f_0\|_{L^{\infty}}$ .

**2.6.** Conclusion of the proof. Optimizing the parameters of the estimates obtained in the previous sections

$$n \sim C_1 |\log \varepsilon|, \quad R^2 \sim C_2 |\log \varepsilon|$$

for some sufficiently large constants  $C_1$  and  $C_2$ , and

$$\delta = \varepsilon^{(d-1)/(d+1)}, \quad \varepsilon_0 = \varepsilon^{d/(d+1)}$$

we find that the total error is smaller than

$$\left\|f^{(s)}(t) - f^{(s)}_N(t)\right\|_{L^{\infty}(K)} \le C\varepsilon^b, \qquad \text{for any } b < \frac{d-1}{d+1}.$$

This ends the proof of Theorem 1.5.

### 3. Long-time asymptotics of a tagged particle

In this section, we sketch the proof of Theorem 1.9 on the diffusive behavior of the tagged particle (see [6] for details of the proof). We shall mainly focus on the first part of Theorem 1.9 which states that the density obeys the heat equation after rescaling. The convergence to the Brownian motion is a strengthening of this result which shows that the rescaled increments of the position become independent in the large N limit.

20

**3.1. Main result.** As explained in the introduction (Theorem 1.7), the heat equation can be recovered from (LB) in some large time limit. Thus our goal is to prove that for an initial data close to equilibrium (15), the time obtained in Lanford's theorem (Theorem 1.5) can be improved up to a time diverging with N and that the solution of the linear Boltzmann equation remains a good approximation of the tagged particle density over such long times. This is the content of the following Theorem from which Theorem 1.9 can be deduced by applying Theorem 1.7.

**Theorem 3.1.** Consider N hard spheres on  $\mathbb{T}^d \times \mathbb{R}^d$ , initially distributed according to (15). Then the distribution  $f_N^{(1)}(t, x, v)$  of the tagged particle is close to the solution  $M_\beta(v)\varphi_\alpha(t, x, v)$  of the linear Boltzmann equation (LB) with initial data  $\rho^0$ , in the sense that for all  $\alpha > 1$ , in the limit  $N \to \infty$ ,  $N\varepsilon^{d-1}\alpha^{-1} = 1$ , one has

$$\left\|f_{N}^{(1)}(t,x,v) - M_{\beta}(v)\varphi_{\alpha}(t,x,v)\right\|_{L^{\infty}([0,\alpha T]\times\mathbb{T}^{d}\times\mathbb{R}^{d})} \le C\left[\frac{T\alpha^{2}}{(\log\log N)^{\frac{A-1}{A}}}\right]^{\frac{A^{2}}{A-1}} (26)$$

where  $A \ge 2$  can be taken arbitrarily large. The constant C depends on A and on the upper bound  $C_0$  on the initial data  $\rho^0$ .

The proof of Theorem 3.1 is the main goal of this section. We shall rely extensively on the arguments used to derive Theorem 1.5 and show that close to equilibrium, they remain valid for macroscopic time scales up to  $o\left(\frac{\log \log N}{\alpha^2}\right)$ . This is achieved by using  $L^{\infty}$  bounds which provide a uniform control in time of the densities and allow us to truncate large collision trees in the Duhamel series.

**3.2. Invariant measure and maximum principle.** Let  $M_{N,\beta}$  be the invariant Gibbs measure for the hard sphere dynamics

$$M_{N,\beta}(Z_N) := \bar{\mathcal{Z}}_N^{-1} \mathbf{1}_{\mathcal{D}_{\varepsilon}^N}(X_N) M_{\beta}^{\otimes N}(V_N), \quad \text{with} \quad \bar{\mathcal{Z}}_N := \int \mathbf{1}_{\mathcal{D}_{\varepsilon}^N}(X_N) \, dX_N.$$

The initial data given by (15) satisfies

$$f_N^0(Z_N) \le C_0 M_{N,\beta} \,.$$

Since  $M_{N,\beta}$  is invariant, the maximum principle implies that this bound remains valid at any time t > 0 and the marginals are uniformly bounded in time

$$\sup_{t} f_{N}^{(s)}(t, Z_{s}) \leq C_{0} M_{N,\beta}^{(s)}(Z_{s}) \leq C_{0} C^{s} M_{\beta}^{\otimes s}(V_{s}),$$

where the last inequality follows from an argument similar to the one leading to (22). Thus the weighted norms (23) are uniformly bounded in time

$$\forall t > 0, \qquad |f_N^{(s)}(t)|_{\varepsilon,s,\beta} \le C_0 C^s.$$
(27)

These bounds are a key step to control the size of the collision trees and to show that large collision trees have vanishing probability. Indeed compared to Section 2.4, these estimates imply a global control of the solution in the space  $\mathbf{X}_{\varepsilon,\beta,\mu}$  with no deterioration on the parameters  $\beta$  and  $\mu = \log C$  with time.

**3.3. Removing large collision trees.** We are going to show that the contribution of large collision trees in the Duhamel series can be neglected. The time interval [0, t] is split into K intervals of time length h, where h is a parameter to be chosen small enough and K = t/h will be large. A collision tree is said to be admissible (see Figure 3) if it has less than  $n_k = A^k$  branching points on the time interval [t - kh, t - (k - 1)h], where A is the constant in the inequality (26), which will be chosen large. The growth of the admissible collision trees is therefore controlled and we are going to show that the other collision trees do not contribute to the Duhamel series.



Figure 3. The collision tree depicted in the figure is not admissible for A = 2 because there are more than  $2^2$  collisions during the second time interval. If the black particles were not involved in the collision tree, then the tree would be admissible.

Defining

$$Q_{s,s+n}(t) := \alpha^n \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} \mathbf{S}_s(t-t_1) C_{s,s+1} \mathbf{S}_{s+1}(t_1-t_2) C_{s+1,s+2} \qquad (28)$$
$$\dots \mathbf{S}_{s+n}(t_n) \, dt_n \dots dt_1 \,,$$

one can write (20) as

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

In particular, the marginal associated to the tagged particle density  $f_N^{(1)}(t)$  can be decomposed as

$$f_N^{(1)}(t) = f_N^{(1,K)}(t) + R_N^K(t), \qquad (29)$$

where the contribution of the admissible trees is

$$f_N^{(1,K)}(t) := \sum_{m_1=0}^{n_1-1} \dots \sum_{m_K=0}^{n_K-1} Q_{1,M_1}(h) Q_{M_1,M_2}(h) \dots Q_{M_{K-1},M_K}(h) f_N^{0(M_K)}$$

and the error term accounts for the contribution of the large trees

$$R_N^K(t) := \sum_{k=1}^K \sum_{m_1=0}^{n_1-1} \dots \sum_{m_{k-1}=0}^{n_{k-1}-1} Q_{1,M_1}(h) \dots Q_{M_{k-2},J_{k-1}}(h)$$
$$R_{M_{k-1},n_k}(t-kh,t-(k-1)h),$$

with

$$R_{k,n}(t',t) := \int_{t'}^{t} \int_{t'}^{t_1} \dots \int_{t'}^{t_{n-1}} \mathbf{T}_k(t-t_1) C_{k,k+1} \mathbf{T}_{k+1}(t_1-t_2) C_{k+1,k+2} \dots \dots C_{k+n-1,k+n} f_N^{(k+n)}(t_n) dt_n \dots dt_1.$$

and where we have defined  $M_k := 1 + \sum_{i=1}^k m_i$ . Note that  $f_N^{(1,K)}(t)$  is evaluated in terms of the initial data, instead in each term of  $R_N^K(t)$  the Duhamel formula is iterated only up to the first time interval [t - kh, t - (k - 1)h] where more than  $n_k = A^k$  collisions occur.

From the upper bound (24) on the collision operator, one can deduce a continuity estimate in terms of the weighted norms (23)

$$\left|Q_{s,s+n}(h)f_{s+n}\right|_{\varepsilon,s,\frac{\beta}{2}} \le e^{s-1} \left(C_{d,\beta} \alpha h\right)^n \left|f_{s+n}\right|_{\varepsilon,s+n,\beta}$$

where  $C_{d,\beta}$  is a constant. The uniform bound in time on the densities (27) enables us to bound from above the collision operators when too many collisions occur on a short time interval h. Choosing  $h = \gamma \alpha^{-A/(A-1)} t^{-1/(A-1)}$ , this leads to an upper bound on the remainder

$$\left\|R_N^K(t)\right\|_{L^{\infty}(\mathbb{T}^d \times \mathbb{R}^d)} \le C\gamma^A \,. \tag{30}$$

Similar computations lead to a similar decomposition for the Boltzmann hierarchy

$$f^{(1)}(t) = f^{(1,K)}(t) + R^{K}(t) \quad \text{with} \quad \left\| R^{K}(t) \right\|_{L^{\infty}(\mathbb{T}^{d} \times \mathbb{R}^{d})} \le C \gamma^{A}.$$
(31)

Thus the dominant contribution in the decompositions (29) and (31) is given by the functions  $f_N^{(1,K)}(t)$  and  $f^{(1,K)}(t)$ . To conclude the proof of Theorem 3.1, it remains to show that  $f_N^{(1,K)}(t)$  and  $f^{(1,K)}(t)$  are close to each other.

**3.4.** Conclusion of the proof of Theorem 3.1. Each term of the sum in  $f_N^{(1,K)}(t)$  can be shown to converge to the corresponding term in  $f^{(1,K)}(t)$  by arguments identical to those developed in Section 2.5 to neglect the influence of the recollisions. Indeed the contribution of a collision tree with *s* collisions in the BBGKY hierarchy will be close to the corresponding contribution in the Boltzmann hierarchy with an error of order  $t^s \varepsilon^b$  (with  $b < \frac{d-1}{d+1}$ ) if no recollision of the pseudo-trajectories occur. This error term is small because the collision trees have been truncated in order to contain less than  $A^K$  particles and *K* can be chosen much smaller than  $\log \log(\varepsilon) / \log A$  by tuning  $\gamma \simeq \frac{(\alpha^2 T)^{A/(A-1)}}{\log \log N}$ . As the remainder  $R_N^K(t)$  in (30) can be controlled as well in terms of  $\gamma$ , the proof of Theorem 3.1 is complete. The parameter *A* can be chosen arbitrarily large.

**3.5.** Convergence to the Brownian motion. We turn now to the second part of Theorem 1.9 and prove the convergence in law of the tagged particle to a Brownian motion.

The first marginal of the Boltzmann hierarchy can be interpreted as the distribution of a single particle  $(\bar{x}(t), \bar{v}(t))$  interacting with an ideal gas at density  $\alpha$  and temperature  $1/\beta$ . This particle changes direction at random times of order  $1/\alpha$ due to collisions. Rephrased in probabilist terms, the velocity  $\{\bar{v}(t)\}_{t\geq 0}$  is a continuous Markov process with generator given by the operator  $\alpha L$  associated to the linear Boltzmann equation. When the density  $\alpha$  of the background gas increases, the frequency of collisions increases by  $\alpha$ . Thus after a time  $\alpha \tau$ , the particle has encountered  $\alpha^2 \tau$  random kicks which is the correct rescaling to observe a diffusive behaviour at the macroscopic scale  $(\tau, x)$  when  $\alpha$  diverges. The position of the tagged particle  $\bar{x}(\alpha \tau) = \bar{x}(0) + \int_0^{\alpha \tau} \bar{v}(s) ds$  is an additive functional of this Markov chain taking values in  $\mathbb{T}^d$ . We consider the rescaled process  $\bar{x}(\alpha \tau)$  taking values in the torus  $\mathbb{T}^d$ . Since L has a spectral gap, the invariance principle holds for the ideal tracer  $\bar{x}(\alpha \tau)$  (see [28] Theorem 2.32 page 74) which converges to a

Brownian motion. The Maxwellian distribution  $M_{\beta}$  is the invariant measure of this process and the diffusion coefficient  $\kappa_{\beta}$  (13) can be recovered as the variance of the position for any coordinate  $k \leq d$ 

$$\kappa_{\beta} = \mathbb{E}_{M_{\beta}} \left[ \bar{v}_k \, L^{-1} \bar{v}_k \right] \, .$$

This implies the convergence of the rescaled finite dimensional marginals towards the ones of the brownian motion B with variance  $\kappa_{\beta}$ , i.e. that for any smooth functions  $\{\psi_i\}_{i < \ell}$  taking values in  $\mathbb{T}^d$  and times  $\tau_1 < \tau_2 < \cdots < \tau_{\ell}$ 

$$\lim_{\alpha \to \infty} \mathbb{E}\Big(\psi_1\big(\bar{x}(\alpha\tau_1)\big) \dots \psi_\ell\big(\bar{x}(\alpha\tau_\ell)\big)\Big) = \mathbb{E}\Big(\psi_1\big(B(\tau_1)\big) \dots \psi_\ell\big(B(\tau_\ell)\big)\Big).$$
(32)

We have shown that the first particle in the Boltzmann hierarchy behaves as a Markov chain. We turn now to the convergence of the rescaled tagged particle  $\Xi(\tau) = x_1(\alpha\tau)$  to a brownian motion when N and  $\alpha \ll \sqrt{\log \log N}$  are diverging (with  $N\varepsilon^{d-1}\alpha^{-1} = 1$ ). For this, one needs to check (see [10]) :

• the convergence of the marginals of the tagged particle sampled at different times  $\tau_1 < \tau_2 < \cdots < \tau_\ell$ 

$$\lim_{N \to \infty} \mathbb{E}\Big(\psi_1\big(\Xi(\tau_1)\big) \dots \psi_\ell\big(\Xi(\tau_\ell)\big)\Big) = \mathbb{E}\Big(\psi_1\big(B(\tau_1)\big) \dots \psi_\ell\big(B(\tau_\ell)\big)\Big).$$
(33)

• the tightness of the sequence, i.e. that is for any  $\tau \in [0, T]$ 

$$\forall \delta > 0, \qquad \lim_{\eta \to 0} \lim_{N \to \infty} \mathbb{P}\left(\sup_{\tau < s < \tau + \eta} \left| \Xi(s) - \Xi(\tau) \right| \ge \delta\right) = 0. \tag{34}$$

We sketch below the main steps for the convergence of the time marginals (33). The tighness follows by similar comparison arguments (see [6]). As for the convergence

of the tagged particle density to the heat equation, we proceed by comparison of the microscopic dynamics with the Boltzmann hierarchy and conclude by using the limit (32). We fix  $\Psi_{\ell} = \{\psi_1, \ldots, \psi_{\ell}\}$  a collection of continuous functions in  $\mathbb{T}^d$ . The density at time t of the tagged particle  $f_{N,\Psi_{\ell}}^{(1)}(t)$  weighted by  $\Psi_{\ell}$  is defined for any test function  $\Phi$  as

$$\int_{\mathbb{T}^d \times \mathbb{R}^d} dZ_1 f_{N, \Psi_\ell}^{(1)}(t, Z_1) \Phi(Z_1(t)) = \mathbb{E}\Big(\psi_1\big(x_1(t_1)\big) \dots \psi_\ell\big(x_1(t_\ell)\big) \Phi(Z_1(t)\big)\Big)$$
$$= \int_{\mathbb{T}^{N^d} \times \mathbb{R}^{N^d}} dZ_N f_N(0, Z_N) \,\psi_1\big(x_1(t_1)\big) \dots \psi_\ell\big(x_1(t_\ell)\big) \Phi(Z_1(t)\big).$$

The Duhamel formula can be applied to rewrite  $f_{N,\Psi_{\ell}}^{(1)}(t)$  as a series

$$f_{N,\Psi_{\ell}}^{(1)}(t) = \sum_{m_{1}+\dots+m_{\ell}=0}^{N-1} Q_{1,1+m_{1}}(t-t_{\ell}) \Big(\psi_{\ell}Q_{1+m_{1},1+m_{1}+m_{2}}(t_{\ell}-t_{\ell-1})\Big(\psi_{\ell-1}\dots Q_{1+m_{1}+\dots+m_{\ell-1},1+m_{1}+\dots+m_{\ell}}(t_{1})\Big) f_{N}^{(m_{1}+\dots+m_{\ell}+1)}(0), \quad (35)$$

where the operator  $Q_{n,m}$  was introduced in (28). Note that this reformulation of the Duhamel series is close in spirit to the one introduced in [30] to encode the trajectory of the tagged particle. An analogous Duhamel formula holds for the density of the first particle in the Boltzmann hierarchy. Thus a coupling of the trajectories in both hierarchies (similar to the one used in section 3.4) shows that

$$\lim_{N\to\infty} \mathbb{E}\Big(\psi_1\big(\bar{x}(\alpha\tau_1)\big)\dots\psi_\ell\big(\bar{x}(\alpha\tau_\ell)\big)\Big) - \mathbb{E}\Big(\psi_1\big(\Xi(\tau_1)\big)\dots\psi_\ell\big(\Xi(\tau_\ell)\big)\Big) = 0.$$

This implies the convergence of the finite dimensional time-marginals (33) and ends the proof of Theorem 1.9.

#### References

- R. Alexander, The Infinite Hard Sphere System, Ph.D. dissertation, Dept. Mathematics, Univ. California, Berkeley, 1975.
- [2] R. Alexander, Time Evolution for Infinitely Many Hard Spheres, Commun. in Math. Phys. 49 (1976), 217-232.
- [3] C. Bardos, R. Santos, R. Sentis, Diffusion approximation and computation of the critical size, *Trans. AMS* (2) 284 (1984), 617-649.
- [4] C. Bardos, S. Ukai, The classical incompressible Navier-Stokes limit of the Boltzmann equation, Math. Models and Methods in the Appl. Sci. 1 (1991), 235-257.
- [5] H. van Beijeren, O.E. III Lanford, J.L Lebowitz, H. Spohn, Equilibrium Time Correlation Functions in the Low Density Limit. *Jour. Stat. Phys.* 22, (1980), 237-257.
- [6] T. Bodineau, I. Gallagher and L. Saint-Raymond, The Brownian motion as the limit of a deterministic system of hard-spheres, *in revision at Inventiones Mathematicae*.

- [7] N. Bogoliubov, Problems of Dynamical Theory in Statistical Physics, in Studies in Statistical Mechanics, J. de Boer and G.E. Uhlenbeck, Ed. Interscience, New York, 1962.
- [8] C. Boldrighini, L.A. Bunimovich, Y. Sinai, On the Boltzmann equation for the Lorentz gas, *Journal of statistical physics*, **32** (3), p. 477-501 (1983).
- [9] M. Born, H. S. Green, A general kinetic theory of liquids. I. The molecular distribution functions, Proc. Roy. Soc. London. Ser. A. 188 (1946), 10-18.
- [10] P. Billingsley, Probability and measure, Wiley Series in Probability and Mathematical Statistics, John Wiley & Sons, 1995.
- [11] L. Bunimovich, Ya. Sinai, Statistical properties of Lorentz gas with periodic configuration of scatterers, Comm. Math. Phys. 78 (4), (1980/81), 479497.
- [12] S. Chapman, T.G. Cowling, The mathematical theory of non-uniform gases: An account of the kinetic theory of viscosity, thermal conduction, and diffusion in gases, Cambridge University Press, New York, 1960.
- [13] C. Cercignani, V. I. Gerasimenko, D. I. Petrina, Many-Particle Dynamics and Kinetic Equations, Kluwer Academic Publishers, Netherlands, 1997.
- [14] C. Cercignani, R. Illner, M. Pulvirenti, The Mathematical Theory of Dilute Gases, Springer Verlag, New York NY, 1994.
- [15] R. DiPerna, P.-L. Lions, On the Cauchy problem for Boltzmann equations: global existence and weak stability, Ann. of Math. (2) 130 (2), (1989), 321-366.
- [16] D. Enskog. Kinetische Theorie der Vorgänge in mässig verdünten Gasen. Uppsala : Almqvist & Wiksell, 1917
- [17] L. Erdös, Lecture notes on quantum Brownian motion, Quantum Theory from Small to Large Scales: Lecture Notes of the Les Houches Summer School, 95, Oxford University Press (2010).
- [18] L. Erdös, M. Salmhofer, H. T. Yau, Quantum diffusion of the random Schrödinger evolution in the scaling limit, Acta mathematica, 200 (2) (2008), 211-278.
- [19] R. Esposito, R. Marra, H.T. Yau. Navier-Stokes equations for stochastic particle systems on the lattice. *Comm. Math. Phys.* 182 (1996), 395-456.
- [20] I. Gallagher, L. Saint-Raymond, B. Texier. From Newton to Boltzmann: the case of hard-spheres and short-range potentials. Zürich Lecture Adv. Math., European Mathematical Society, 2013.
- [21] G. Gallavotti. Rigorous theory of the Boltzmann equation in the Lorentz gas. Università di Roma, Instituto di Fisica, Nota Interna 358 (1972).
- [22] F. Golse, L. Saint-Raymond. The Incompressible Navier-Stokes Limit of the Boltzmann Equation for Hard Cutoff Potentials, J. Math. Pures Appl. 91 (2009), 508-552.
- [23] H. Grad, On the kinetic theory of rarefied gases, Comm. Pure Appl. Math. 2 (1949), 331-407.
- [24] H. Grad. Asymptotic theory of the Boltzmann equation II Rarefied Gas Dynamics (Proc. of the 3rd Intern. Sympos. Palais de l'UNESCO, Paris, 1962) Vol. I, 26–59.
- [25] D. Hilbert, Sur les problèmes futurs des mathématiques, in Compte-Rendu du 2ème Congrès International de Mathématiques, Gauthier-Villars, Paris (1902), 58-114.
- [26] D. Hilbert. Begründung der kinetischen Gastheorie Math. Ann. 72 (1912), 562-577.

- [27] J. G. Kirkwood, The Statistical Mechanical Theory of Transport Processes I. General Theory, *Journal of Chemical Physics* 14 (1946) 180-202.
- [28] T. Komorowski, C. Landim, S. Olla, Fluctuations in Markov processes. Time symmetry and martingale approximation, Grundlehren der Mathematischen Wissenschaften, 345 Springer, Heidelberg, 2012.
- [29] O.E. Lanford, *Time evolution of large classical systems*, Lect. Notes in Physics 38, J. Moser ed., 1-111, Springer Verlag (1975).
- [30] J. Lebowitz, H. Spohn, Steady state self-diffusion at low density. J. Statist. Phys. 29 (1982), 39-55.
- [31] J. Lukkarinen, H. Spohn, Weakly nonlinear Schrödinger equation with random initial data, *Inventiones mathematicae* 183 (1), (2011), 79-188.
- [32] J. Marklof, Kinetic transport in crystals, Proceedings of the XVI International Congress on Mathematical Physics, Prague 2009, World Scientific 2010, 162–179.
- [33] T. Nishida. Fluid dynamical limit of the nonlinear Boltzmann equation to the level of the compressible Euler equation. *Comm. Math. Phys.* **61** (1978), 119-148.
- [34] T. Nishida, A note on a theorem by Nirenberg, Journal of Differential Geometry, 12 (1977), 629-633.
- [35] S. Olla, S. Varadhan, H.-T. Yau, Hydrodynamical limit for a Hamiltonian system with weak noise, *Commun. Math. Phys.* 155 (1993), 523-560.
- [36] G. Papanicolaou, Asymptotic analysis of transport processes, Bull. AMS 81 (1975), 330-392.
- [37] M. Pulvirenti, C. Saffirio, S. Simonella, On the validity of the Boltzmann equation for short range potentials, arXiv:1301.2514.
- [38] J. Quastel, H.-T. Yau, Lattice gases, large deviations, and the incompressible Navier-Stokes equations, Ann. of Math. 148 (1998), 51-108.
- [39] L. Saint-Raymond, Hydrodynamic limits of the Boltzmann equation, Lecture Notes in Mathematics, Springer-Verlag 1971, 2009.
- [40] S. Simonella, Evolution of correlation functions in the hard sphere dynamics, arXiv:1205.2789
- [41] H. Spohn, Large scale dynamics of interacting particles, Springer-Verlag 174, 1991.
- [42] K. Uchiyama, Derivation of the Boltzmann equation from particle dynamics, *Hiroshima Math. J.* 18 (1988), no. 2, p. 245-297.
- [43] S. Ukai, The Boltzmann-Grad Limit and Cauchy-Kovalevskaya Theorem, Japan J. Indust. Appl. Math. 18 (2001), 383-392.
- [44] C. Villani, Limites hydrodynamiques de l'équation de Boltzmann, Sém. Bourbaki 2000/01, Exp 893, Astérisque 282 (2002), 365-405.
- [45] J. Yvon, La théorie statistique des fluides et l'équation d'état, Actual. Sci. et Indust.
   203 (Paris, Hermann), 1935.

1. CNRS & École Polytechnique, Centre de Mathématiques Appliquées E-mail: Thierry.Bodineau@polytechnique.edu 2. Université Paris-Diderot, Institut de Mathématiques de Jussieu-Paris Rive Gauche E-mail: gallagher@math.univ-paris-diderot.fr

3. Université Pierre et Marie Curie & École Normale Supérieure, Département de Mathématiques et Applications
 E-mail: Laure.Saint-Raymond@ens.fr