

On the dynamics of dilute gases

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The evolution of a gas can be described by different mathematical models depending on the scale of observation. A natural question, raised by Hilbert in his sixth problem, is whether these models provide mutually consistent predictions. In particular, for rarefied gases, it is expected that the equations of the kinetic theory of gases can be obtained from molecular dynamics governed by the fundamental principles of mechanics. In the case of hard sphere gases, Lanford (1975) has shown that the Boltzmann equation does indeed appear as a law of large numbers in the low density limit, at least for very short times. The aim of this paper is to present recent advances in the understanding of this limiting process.

1 A statistical approach to dilute gas dynamics

1.1 The physical model: A dilute gas of hard spheres

Although at the time Boltzmann published his famous paper [8] the atomic theory was still rejected by some scientists, it was already well established that matter is composed of atoms, which are the elementary constituents of all solids, liquids and gases. The particularity of gases is that the volume occupied by their atoms is negligible as compared to the total volume occupied by the gas, and there are therefore very few constraints on the atoms' geometric arrangement: they are thus very loosely bound and almost independent. Neglecting the internal structure of the atoms, their possible organization into molecules, and the effect of long-range interactions, a gas can be represented as a system formed by a large number of particles that move in a straight line and occasionally collide with each other, resulting in an almost instantaneous scattering. The simplest example of such a model consists in assuming that the particles are small identical spheres, of diameter $\varepsilon \ll 1$ and mass 1, interacting only by contact (Figure 1). We refer to this as a *gas of hard spheres*. This microscopic description of a gas is explicit, but very difficult to use in practice because the number of particles is extremely large, their size is tiny and their collisions are very sensitive to small shifts (Figure 2). This model is therefore not efficient for making theoretical predictions. A natural question is whether one can extract, from such a complex system, less precise but more stable models suitable for applications, such

as kinetic or fluid models. This question was formalized by Hilbert at the International Congress of Mathematicians in 1900, in his sixth problem:

Boltzmann's work on the principles of mechanics suggests the problem of developing mathematically the limiting processes, there merely indicated, which lead from the atomistic view to the laws of motion of continua.

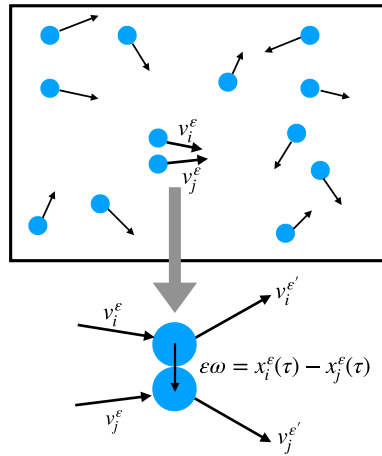
The Boltzmann equation, mentioned by Hilbert and described in more detail below, expresses that the particle distribution evolves under the combined effect of free transport and collisions. For these two effects to be of the same order of magnitude, a simple calculation shows that, in dimension $d \geq 2$, the number of particles N and their diameter ε must satisfy the scaling relation $N\varepsilon^{d-1} = O(1)$, called *low density scaling* [14]. Indeed, the regime described by the Boltzmann equation is such that the mean free path, i.e., the average distance traveled by a particle moving in a straight line between two collisions, is of order 1. Thus, a typical particle should go through a tube of volume $O(\varepsilon^{d-1})$ between two collisions, and on average, this tube should cross one of the $N - 1$ other particles. Note that, in this regime, the total volume occupied by the particles at a given time is proportional to $N\varepsilon^d$ and is therefore negligible compared to the total volume occupied by the gas. We speak then of a *dilute gas*.

1.2 Three levels of averaging

Henceforth, it is assumed that the particle system evolves in the unit domain with periodic boundary conditions $\mathbb{T}^d = [0, 1]^d$. We consider that the N particles are identical: this is the exchangeability assumption. The state of the system can be represented by a measure in the phase space $\mathbb{T}^d \times \mathbb{R}^d$ called *empirical measure*,

$$\frac{1}{N} \sum_{i=1}^N \delta_{x-x_i} \delta_{v-v_i},$$

where δ_x is the Dirac mass at $x = 0$. This measure is completely symmetric (i.e., invariant under permutation of the indices of the particles) because of the exchangeability assumption. This first aver-



Hard sphere dynamics:

$$\frac{dx_k^\epsilon}{dt} = v_k^\epsilon, \quad \frac{dv_k^\epsilon}{dt} = 0$$

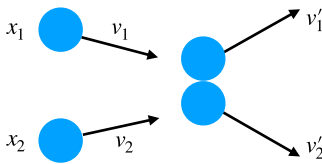
as long as

$$|x_k^\epsilon(t) - x_{k'}^\epsilon(t)| > \epsilon, \quad 1 \leq k \neq k' \leq N$$

$$\begin{aligned} v_i^{\epsilon'} &= v_i^\epsilon - ((v_i^\epsilon - v_j^\epsilon) \cdot \omega) \omega, \\ v_j^{\epsilon'} &= v_j^\epsilon + ((v_i^\epsilon - v_j^\epsilon) \cdot \omega) \omega \end{aligned}$$

Figure 1. At time t , the system of hard spheres is described by the positions $(x_k^\epsilon(t))_{k \leq N}$ and the velocities $(v_k^\epsilon(t))_{k \leq N}$ of the centers of gravity of the particles. The spheres move in a straight line and when two of them touch, they are scattered according to elastic reflection laws.

Case 1: transport and collision (the velocities are scattered)



Case 2: free transport (the particles do not collide)

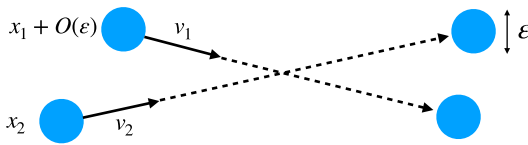


Figure 2. The particles are very small (of diameter $\epsilon \ll 1$) and the dynamics is very sensitive to small spatial shifts. In the first case depicted above, two particles with initial positions x_1, x_2 and velocities v_1, v_2 collide and are scattered. In the second case, after shifting the position of the first particle by a distance $O(\epsilon)$, they no longer collide and each particle keeps moving in a straight line. Thus, a perturbation of order ϵ of the initial conditions can lead to very different trajectories.

aging is however not sufficient to obtain a robust description of the dynamics when N is large, because of the instabilities mentioned in the previous section (Figure 2) which lead to a strong dependence of the particle trajectories on ϵ .

We will therefore introduce a second averaging, with respect to the initial configurations; from a physical point of view, this averaging is natural since only fragmentary information on the initial configuration is available. We therefore assume that the initial data $(X_N, V_N) = (x_i, v_i)_{1 \leq i \leq N}$ are independent random variables, identically distributed according to a distribution $f^0 = f^0(x, v)$. This

assumption must be slightly corrected to account for particle exclusion: $|x_i - x_j| > \epsilon$ for $i \neq j$. This statistical framework is called the *canonical* setting. It is a simple framework allowing us to establish rigorous foundations for the kinetic theory, i.e., to characterize, in the large N asymptotics, the average dynamics and more precisely the evolution equation governing the distribution $f(t, x, v)$ at time t of a typical particle.

In this paper, our aim is to go beyond this averaged dynamics, and to describe in a precise way the correlations that appear dynamically inside the gas. Fixing a priori the number N of particles induces additional correlations, so to circumvent them, we introduce a third level of averaging by assuming that N is also a random variable, and that only its average $\mu_\epsilon = \epsilon^{-(d-1)}$ is determined (according to the low density scaling). To define a system of initially independent (modulo exclusion) identically distributed hard spheres according to f^0 , we introduce the *grand canonical* measure as follows: the probability density of finding N particles of coordinates $(x_i, v_i)_{i \leq N}$ is given by

$$\frac{1}{Z^\epsilon} \frac{\mu_\epsilon^N}{N!} \prod_{i=1}^N f^0(x_i, v_i) \prod_{i \neq j} \mathbf{1}_{|x_i - x_j| > \epsilon} \quad \text{for } N = 0, 1, 2, \dots, \quad (1.1)$$

where the constant Z^ϵ is the normalization factor of the probability measure. We will assume in the following that the function f^0 is Lipschitz continuous, with a Gaussian decay in velocity. The corresponding probability and expectation will be denoted by \mathbb{P}_ϵ and \mathbb{E}_ϵ .

1.3 A statistical approach

Once the initial random configuration $(N, (x_i^{\epsilon 0}, v_i^{\epsilon 0})_{1 \leq i \leq N})$ is chosen, the hard sphere dynamics evolves deterministically (according to the hard sphere equations shown in Figure 1), and we seek to

understand the statistical behavior of the empirical measure

$$\pi_t^\varepsilon(x, \nu) := \frac{1}{\mu_\varepsilon} \sum_{i=1}^N \delta_{x-x_i^\varepsilon(t)} \delta_{\nu-\nu_i^\varepsilon(t)} \quad (1.2)$$

and its evolution in time.

A law of large numbers

The first step is to determine the law of large numbers, that is, the limiting distribution of a typical particle when $\mu_\varepsilon \rightarrow \infty$. In the case of N identically distributed independent variables $(\eta_i)_{1 \leq i \leq N}$ of expectation $\mathbb{E}(\eta)$, the law of large numbers implies in particular that the mean converges in probability to the expectation:

$$\frac{1}{N} \sum_{i=1}^N \eta_i \xrightarrow[N \rightarrow \infty]{} \mathbb{E}(\eta).$$

One can easily show the following convergence in probability:

$$\langle \pi_0^\varepsilon, h \rangle := \frac{1}{\mu_\varepsilon} \sum_{i=1}^N h(x_i^{\varepsilon 0}, \nu_i^{\varepsilon 0}) \xrightarrow[\mu_\varepsilon \rightarrow \infty]{} \int f^0 h(x, \nu) dx d\nu,$$

under the grand canonical measure. The difficulty is to understand whether the initial quasi-independence propagates in time so that there exists a function $f = f(t, x, \nu)$ such that the following convergence in probability holds:

$$\langle \pi_t^\varepsilon, h \rangle \xrightarrow[\mu_\varepsilon \rightarrow \infty]{} \int f(t, x, \nu) h(x, \nu) dx d\nu \quad (1.3)$$

under the grand canonical measure (1.1) over the initial configurations. The most important result proving this convergence was obtained by Lanford [16]: he showed that f evolves according to a deterministic equation, namely the Boltzmann equation. This result will be explained in Section 2.2.

A central limit theorem

The approximation (1.3) of the empirical measure neglects two types of errors. The first is the presence of correction terms that converge to 0 when $\mu_\varepsilon \rightarrow +\infty$. The second is related to the probability, which must tend to zero, of configurations for which this convergence does not occur. A classical problem in statistical physics is to quantify more precisely these errors, by studying the fluctuations, i.e., the deviations between the empirical measure and its expectation. In the case of N independent and identically distributed variables $(\eta_i)_{1 \leq i \leq N}$, the central limit theorem implies that the fluctuations are of order $O(1/\sqrt{N})$, and the following convergence in law holds true:

$$\sqrt{N} \left(\frac{1}{N} \sum_{i=1}^N \eta_i - \mathbb{E}(\eta) \right) \xrightarrow[N \rightarrow \infty]{(\text{law})} \mathcal{N}(0, \text{Var}(\eta)),$$

where $\mathcal{N}(0, \text{Var}(\eta))$ is the normal law of variance $\text{Var}(\eta) = \mathbb{E}((\eta - \mathbb{E}(\eta))^2)$. In particular, at this scale, we find some randomness. Investigating the same fluctuation regime for the dynamics of hard sphere gases consists in considering the fluctuation field ζ_t^ε defined

by duality, namely,

$$\langle \zeta_t^\varepsilon, h \rangle := \sqrt{\mu_\varepsilon} (\langle \pi_t^\varepsilon, h \rangle - \mathbb{E}_\varepsilon(\langle \pi_t^\varepsilon, h \rangle)), \quad (1.4)$$

where h is a continuous function, and \mathbb{E}_ε the expectation with respect to the grand canonical measure. At time 0, one can easily show that, under the grand-canonical measure, the fluctuation field ζ_0^ε converges in the low density limit to a Gaussian field ζ_0 with covariance

$$\mathbb{E}(\zeta_0(h)\zeta_0(g)) = \int f^0(z)h(z)g(z) dz.$$

A series of recent works [4–7] has allowed to characterize the fluctuation field (1.4) and to obtain a stochastic evolution equation governing the limit process. These results are presented in Section 3.3.

On large deviations

The last question generally studied in a classical probabilistic approach is that of the quantification of rare events, i.e., the estimation of the probability of observing an atypical behavior (which deviates macroscopically from the mean). For independent and identically distributed random variables, this probability is exponentially small, and it is therefore natural to study the asymptotics

$$I(m) := \lim_{\delta \rightarrow 0} \lim_{N \rightarrow \infty} -\frac{1}{N} \log \mathbb{P} \left(\left| \frac{1}{N} \sum_{i=1}^N \eta_i - m \right| < \delta \right) \quad \text{with } m \neq \mathbb{E}(\eta).$$

The limit $I(m)$ is called the large deviation functional and can be expressed as the Legendre transform of the log-Laplace transform $\mathbb{R} \ni u \mapsto \log \mathbb{E}(\exp(u\eta))$. To generalize this statement to correlated variables in a gas of hard spheres, it is necessary to compute the log-Laplace transform of the empirical measure on deterministic trajectories, which requires extremely precise control of the dynamical correlations. Note that, at time 0, under the grand canonical measure, one can show that, for any $\delta > 0$,

$$\begin{aligned} \lim_{\delta \rightarrow 0} \lim_{\mu_\varepsilon \rightarrow \infty} -\frac{1}{\mu_\varepsilon} \log \mathbb{P}_\varepsilon(d(\pi_0^\varepsilon, \varphi^0) \leq \delta) \\ = H(\varphi^0 | f^0) := \int \left(\varphi^0 \log \frac{\varphi^0}{f^0} - (\varphi^0 - f^0) \right) dx d\nu, \end{aligned}$$

where d is a distance on the space of measures. The dynamical cumulant method introduced in [4, 6] is a key tool for computing the exponential moments of the hard sphere distribution, thus obtaining the dynamical equivalent of this result in short time. We give an overview of these techniques in Section 3.

2 Typical behavior: A law of large numbers

2.1 Boltzmann's amazing intuition

The equation that rules the typical evolution of a gas of hard spheres was heuristically proposed by Boltzmann [8] about a century before

its rigorous derivation by Lanford [16], as the “limit” of the particle system when $\mu_\varepsilon \rightarrow +\infty$. Boltzmann’s revolutionary idea was to write an evolution equation for the probability density $f = f(t, x, v)$ giving the proportion of particles at position x with velocity v at time t . In the absence of collisions, and in an unbounded domain, this density f would be transported along the physical trajectories $x(t) = x(0) + vt$, which means that $f(t, x, v) = f^0(x - vt, v)$. The challenge is to take into account the statistical effect of collisions. As long as the size of the particles is negligible, one can consider that these collisions are pointwise in both t and x . Boltzmann proposed a quite intuitive counting:

- the number of particles of velocity v increases when a particle of velocity v' collides with a particle of velocity v'_1 , and takes the velocity v (Figure 1 and (2.2));
- the number of particles of velocity v decreases when a particle of velocity v collides with a particle of velocity v_1 , and is deflected to another velocity.

The probability of these jumps in velocity is described by a transition rate, called the *collision cross section*. For interactions between hard spheres, it is given by $((v - v_1) \cdot \omega)_+$, where $v - v_1$ is the relative velocity of the colliding particles, and ω is the deflection vector, uniformly distributed in the unit sphere $\mathbb{S}^{d-1} \subset \mathbb{R}^d$.

The fundamental assumption of Boltzmann’s theory is that, in a rarefied gas, the correlations between two colliding particles must be very small. Therefore, the joint probability of having two pre-colliding particles of velocities v and v_1 at position x at time t should be well approximated by the product $f(t, x, v)f(t, x, v_1)$. This independence property is called the *molecular chaos hypothesis*. The Boltzmann equation then reads

$$\partial_t f + \underbrace{v \cdot \nabla_x f}_{\text{transport}} = \underbrace{C(f, f)}_{\text{collision}}, \quad (2.1)$$

where

$$C(f, f)(t, x, v) = \iint \underbrace{[f(t, x, v')f(t, x, v'_1)]}_{\text{gain term}} - \underbrace{[f(t, x, v)f(t, x, v_1)]}_{\text{loss term}} \times \underbrace{((v - v_1) \cdot \omega)_+}_{\text{cross section}} dv_1 d\omega,$$

with the scattering rules

$$v' = v - ((v - v_1) \cdot \omega)\omega, \quad v'_1 = v_1 + ((v - v_1) \cdot \omega)\omega \quad (2.2)$$

being analogous to those introduced in Figure 1, with the important difference that ω is now a random vector chosen uniformly in the unit sphere \mathbb{S}^{d-1} : indeed, the relative position of the colliding particles disappeared in the limit $\varepsilon \rightarrow 0$. As a result, the Boltzmann equation is singular because it involves a product of densities at a single point x .

Boltzmann’s idea of reducing the Hamiltonian dynamics describing atomic behavior to a kinetic equation was revolutionary and paved the way to the description of non-equilibrium phenomena by mesoscopic equations. However, the Boltzmann equation

(2.1) was first strongly criticized because it seems to violate some fundamental physical principles. It actually predicts an irreversible evolution in time: it has a Lyapunov functional, called entropy, defined by $S(t) := - \iint f \log f(t, x, v) dx dv$, such that $\frac{d}{dt} S(t) \geq 0$, with equality if and only if the gas is in thermodynamic equilibrium. The Boltzmann equation thus provides a quantitative formulation of the second principle of thermodynamics. But at first glance, this irreversibility seems incompatible with the fact that the dynamics of hard spheres is governed by a Hamiltonian system, i.e., a system of ordinary differential equations that is completely reversible in time. Soon after Boltzmann postulated his equation, these two different behaviors were considered, by Loschmidt, as a paradox and an obstruction to Boltzmann’s theory. A fully satisfactory mathematical explanation of this question remained elusive for almost a century, until the role of probabilities was precisely identified: the underlying dynamics is reversible, but the description that is given of this dynamics is only partial and is therefore not reversible.

2.2 Typical behavior: Lanford’s theorem

Lanford’s result [16] shows in which sense the Boltzmann equation (2.1) is a good approximation of the hard sphere dynamics. It can be stated as follows (this is not exactly the original formulation; see in particular Section 2.4 below for comments).

Theorem 2.1 (Lanford). *In the low density limit ($\mu_\varepsilon \rightarrow \infty$ with $\mu_\varepsilon \varepsilon^{d-1} = 1$), the empirical measure π_ε^ξ defined by (1.2) concentrates on the solution of the Boltzmann equation (2.1): for any bounded and continuous function h ,*

$$\forall \delta > 0, \quad \lim_{\mu_\varepsilon \rightarrow \infty} \mathbb{P}_\varepsilon \left(\left| \langle \pi_\varepsilon^\xi, h \rangle - \int f(t, x, v) h(x, v) dx dv \right| \geq \delta \right) = 0,$$

on a time interval $[0, T_L]$ that depends only on the initial distribution f^0 .

The time of validity T_L of the approximation is found to be a fraction of the average time between two successive collisions for a typical particle. This time is large enough for the microscopic system to undergo a large number of collisions (of the order of μ_ε), but (much) too small to see phenomena such as relaxation to (local) thermodynamic equilibrium, and in particular hydrodynamic regimes. Physically, we do not expect this time to be critical, in the sense that the dynamics would change in nature afterwards. In fact, in practice, Boltzmann’s equation is used in many applications (such as spacecraft reentrance calculations) without time restrictions. However, it is important to note that a time restriction might not be only technical: from a mathematical point of view, one cannot exclude that the Boltzmann equation presents singularities (typically spatial concentrations that would prevent the collision term from making sense, and that would also locally contradict the low density assumption). At present, the problem of

extending Lanford's convergence result to longer times still faces serious obstacles.

2.3 Heuristics of Lanford's proof

Let us informally explain how the Boltzmann equation (2.1) can be predicted from the dynamics of the particles. The goal is to transport via the dynamics the initial grand canonical measure (1.1) and then to project this measure at time t onto the 1-particle phase space. We thus define by duality the density $F_1^\varepsilon(t, x, v)$ of a typical particle with respect to a test function h by

$$\int F_1^\varepsilon(t, x, v)h(x, v) dx dv := \mathbb{E}_\varepsilon(\langle \pi_t^\varepsilon, h \rangle). \quad (2.3)$$

Theorem 2.1 states that F_1^ε converges to the solution to the Boltzmann equation f in the low density limit. So let h be a regular and bounded function on $\mathbb{T}^d \times \mathbb{R}^d$ and consider the evolution of the empirical measure during a short time interval $[t, t + \delta]$. Separating the different contributions according to the number of collisions, we can write

$$\begin{aligned} & \frac{1}{\delta} (\mathbb{E}_\varepsilon[\langle \pi_{t+\delta}^\varepsilon, h \rangle] - \mathbb{E}_\varepsilon[\langle \pi_t^\varepsilon, h \rangle]) \\ &= \frac{1}{\delta} \mathbb{E}_\varepsilon \left[\frac{1}{\mu_\varepsilon} \sum_{\text{no collision}} (h(z_j^\varepsilon(t + \delta)) - h(z_j^\varepsilon(t))) \right] \\ &+ \frac{1}{\delta} \mathbb{E}_\varepsilon \left[\frac{1}{2\mu_\varepsilon} \sum_{\substack{(i,j) \\ \text{one collision}}} (h(z_i^\varepsilon(t + \delta)) + h(z_j^\varepsilon(t + \delta)) \right. \\ &\quad \left. - h(z_i^\varepsilon(t)) - h(z_j^\varepsilon(t))) \right] \\ &+ \dots \end{aligned} \quad (2.4)$$

To simplify, $z_j^\varepsilon(t)$ denotes the coordinates $(x_j^\varepsilon(t), v_j^\varepsilon(t))$ of the j -th particle at time t . Since the left-hand side of (2.4) formally converges when $\delta \rightarrow 0$ to the time derivative of $\mathbb{E}_\varepsilon[\langle \pi_t^\varepsilon, h \rangle]$, we will analyze the limit $\delta \rightarrow 0$ of the first two terms in the right-hand side of (2.4), which should lead to a transport term and a collision term as in (2.1). We will also explain why the remainder terms, involving two or more collisions in the short time interval δ , tend to 0 with δ (showing that they are of order δ).

Since the particles move in a straight line and at constant speed in the absence of collisions, if the distribution F_1^ε is sufficiently regular, the definition (2.3) of F_1^ε formally implies that, when δ tends to 0, the first term in the right-hand side of (2.4) is asymptotically equal to

$$\int F_1^\varepsilon(t, z)v \cdot \nabla_x h(z) dz = - \int (v \cdot \nabla_x F_1^\varepsilon(t, z))h(z) dz.$$

The transport term in (2.1) is thus well obtained in the limit. Let us now consider the second term in the right-hand side of (2.4). Two particles of configurations (x_1, v_1) and (x_2, v_2) at time t collide at a later time $\tau \leq t + \delta$ if there exists $\omega \in \mathbb{S}^{d-1}$ such that

$$x_1 - x_2 + (\tau - t)(v_1 - v_2) = -\varepsilon\omega. \quad (2.5)$$

This implies that their relative position must belong to a tube of length $\delta|v_1 - v_2|$ and width ε oriented in the $v_1 - v_2$ direction. The Lebesgue measure of this set is of the order $\delta\varepsilon^{d-1}|v_2 - v_1| = O(\delta\varepsilon^{d-1})$ (neglecting large velocities). More generally, a sequence of $k - 1$ collisions between k particles imposes $k - 1$ constraints of the previous form, and this event can be shown to have probability less than $(\delta\varepsilon^{d-1})^{k-1} = (\delta\mu_\varepsilon^{-1})^{k-1}$ (again neglecting large velocities). Since there are, on average, μ_ε^k ways to choose these k colliding particles, we deduce that the occurrence of $k - 1$ collisions in (2.4) has a probability of order $\delta^{k-1}\mu_\varepsilon$. This explains why the probability of having $k \geq 3$ colliding particles can be estimated by $O(\delta^2)$ and thus can be neglected in (2.4).

It remains to examine more closely the collision term involving two particles in (2.4), in order to obtain the collision operator $C(f, f)$ of the Boltzmann equation (2.1). This term involves the two-particle correlation function F_2^ε . For any $k \geq 1$, we define

$$\begin{aligned} & \int F_k^\varepsilon(t, Z_k)h_k(Z_k) dZ_k \\ &= \mathbb{E}_\varepsilon \left(\frac{1}{\mu_\varepsilon^k} \sum_{(i_1, \dots, i_k)} h_k(z_{i_1}^\varepsilon(t), \dots, z_{i_k}^\varepsilon(t)) \right), \end{aligned} \quad (2.6)$$

where i_1, \dots, i_k are all distinct and $Z_k = (x_i, v_i)_{1 \leq i \leq k}$. We can then show that, in the limit $\delta \rightarrow 0$,

$$\partial_t F_1^\varepsilon + \underbrace{v \cdot \nabla_x F_1^\varepsilon}_{\text{transport}} = \underbrace{C^\varepsilon(F_2^\varepsilon)}_{\text{collision at distance } \varepsilon}, \quad (2.7)$$

where

$$\begin{aligned} & C^\varepsilon(F_2^\varepsilon)(t, x, v) \\ &= \iint \underbrace{[F_2^\varepsilon(t, x, v', x + \varepsilon\omega, v')]}_{\text{gain term}} - \underbrace{F_2^\varepsilon(t, x, v, x - \varepsilon\omega, v_1)}_{\text{loss term}} \\ &\quad \times \underbrace{((v - v_1) \cdot \omega)_+}_{\text{cross section}} dv_1 d\omega. \end{aligned}$$

The key step in closing the equation is the *molecular chaos assumption* postulated by Boltzmann, which states that the pre-collisional particles remain independently distributed at all times so that, with the convention (2.5) fixing the sign of ω , we have

$$F_2^\varepsilon(t, z_1, z_2) \simeq F_1^\varepsilon(t, z_1)F_1^\varepsilon(t, z_2) \quad \text{if } (v_1 - v_2) \cdot \omega > 0. \quad (2.8)$$

When the diameter ε of the spheres tends to 0, the coordinates x_1 and x_2 coincide and the scattering parameter ω becomes a random parameter. Assuming that F_1^ε converges, its limit must satisfy the Boltzmann equation (2.1).

Establishing the factorization (2.8) rigorously uses a different strategy, elaborated by Lanford [16], then completed and improved over the years: see the monographs [10, 11, 25]. In the last few years, several quantitative convergence results have been established, and the proofs have been extended to the case of somewhat more general domains, potentials with compact support, or with super-exponential decay at infinity: see [1, 12, 13, 17, 21, 22].

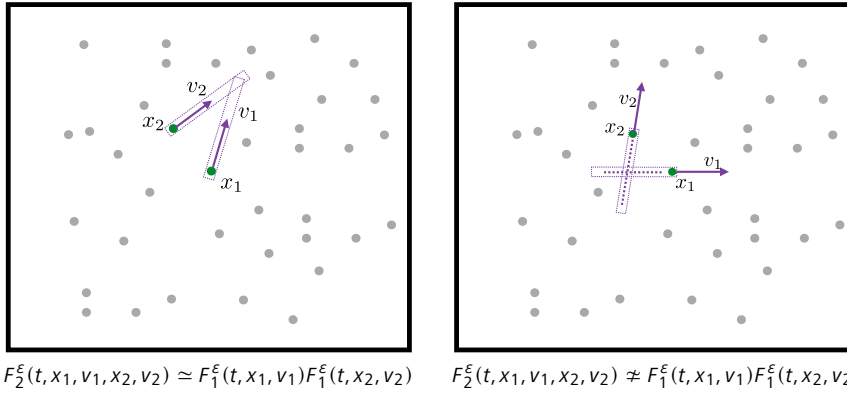


Figure 3. In the left figure, particles 1 and 2 will meet in the future; with high probability, they did not collide in the past and we expect the correlation function F_2^ϵ to factorize in the $\mu_\epsilon \rightarrow \infty$ limit. In the figure on the right, the coordinates of the particles belong to the bad set \mathcal{B}_2^ϵ , which means that they most likely met in the past. In this case, microscopic correlations have been dynamically constructed and the factorization (2.8) should not be valid.

2.4 On the irreversibility

In this section, we will show that the answer to the irreversibility paradox lies in the molecular chaos hypothesis (2.8), which is valid only for specific configurations.

In fact, the notion of convergence that appears in the statement of Theorem 2.1 differs from the one used in Lanford's proof: Theorem 2.1 states the convergence of the $\langle \pi_t^\epsilon, h \rangle$ observables, i.e., the convergence in the sense of measures, since the test function h must be continuous. This convergence is rather weak and is not sufficient to ensure the stability of the collision term in the Boltzmann equation because this term involves traces. In the proof of Lanford's theorem, we consider all k -particle correlation functions F_k^ϵ defined by (2.6) and show that, when $\mu_\epsilon \rightarrow \infty$, each of these correlation functions converges uniformly outside a set \mathcal{B}_k^ϵ of negligible measure. Thus, the proof uses a much stronger notion of convergence than that stated in Theorem 2.1. Moreover, the set \mathcal{B}_k^ϵ of bad microscopic configurations (t, Z_k) (on which F_k^ϵ does not converge) is somehow transverse to the set of pre-collisional configurations (as can be seen in Figure 3; two particles in \mathcal{B}_2^ϵ tend to move away from each other so that they are unlikely to collide). The convergence defect is therefore not an obstacle to taking bounds in the collision term (correlation functions are only evaluated there in pre-collisional configurations). However, these singular sets \mathcal{B}_k^ϵ encode important information about the dynamical correlations: by neglecting them, it is no longer possible to go back in time and reconstruct the backward dynamics. Thus, by discarding the microscopic information encoded in \mathcal{B}_k^ϵ , one can only obtain an irreversible kinetic picture that is far from describing the full microscopic dynamics.

3 Fluctuations and large deviations

3.1 Corrections to the chaos assumption

Returning to equation (2.7) on F_1^ϵ , we can see that, apart from the small spatial shifts of the collision term, the deviations of the Boltzmann dynamics are due to the factorization defect $F_2^\epsilon - F_1^\epsilon \otimes F_1^\epsilon$, a geometric interpretation of which is given below.

Let us first describe the geometric representation of F_1^ϵ . We look at the history of particle 1^* located at position x_{1^*} with velocity v_{1^*} at time t , in order to characterize all initial configurations that contribute to $F_1^\epsilon(t, x_{1^*}, v_{1^*})$. The particle 1^* performs a uniform rectilinear motion $x_{1^*}(t') = x_{1^*} - v_{1^*}(t - t')$ until it collides with another particle, called particle 1, at a time $t_1 < t$. This collision can be of two types: either a physical collision (with deflection), or a mathematical artifact arising from the loss term in equation (2.7)

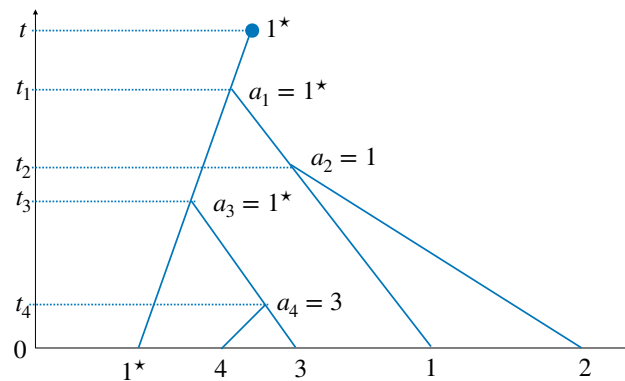


Figure 4. The history of the particle 1^* can be encoded in a tree a , say of size n , whose root is indexed by 1^* . The pseudotrajectory is then prescribed by the collision parameters $(t_i, v_i, \omega_i)_{1 \leq i \leq n}$.

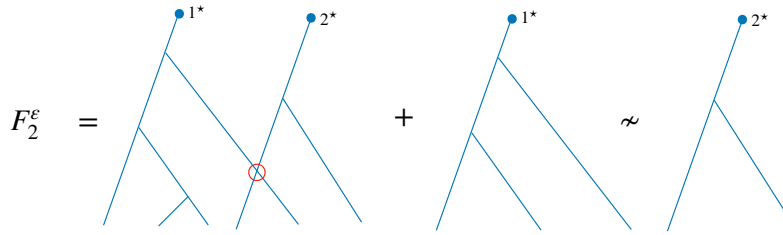


Figure 5. F_2^ϵ trees are classified into two categories: those involving an (external) collision between the 1^* and 2^* trees, and others for which the particles in the 1^* tree are always at least ϵ away from those in the 2^* tree (which we denote by \rightsquigarrow).

(the particles touch but are not deflected). From then on, to understand the history of particle 1^* , we need to trace the history of both particles 1^* and 1 before time t_1 . From time t_1 on, both particles perform uniform rectilinear motions until one of them collides with a new particle 2 at time $t_2 < t_1$, and so on, until time 0. Note that, between the times of collision with new particles, the particles can collide with each other: this will be called *recollision*. The history of the particle 1^* can be encoded using a rooted tree a whose vertices correspond to the different collisions that took place in the history of 1^* and are indexed by the parameters of these collisions. An example is shown in Figure 4. The root of the tree a is indexed by 1^* . If n is the total number of collisions, and $0 < t_n < \dots < t_1 < t$ are the times of the collisions, one can order the particles so that, at time t_i , $1 \leq i \leq n$, the collision occurs between the i -th particle and the j -th particle, where $j \in \{1^*, 1, \dots, i-1\}$ (necessarily, $j = 1^*$ at time t_1). Then the branching of the tree a associated with the i -th collision is indexed by the relation $a_i = j$, where $j \in \{1^*, 1, \dots, i-1\}$, together with the collision parameters $(t_i, v_i, \omega_i)_{1 \leq i \leq n}$, where ω_i is the deflection vector. The tensor product $F_1^\epsilon \otimes F_1^\epsilon$ is then described by two independent collision trees, with roots 1^* and 2^* , and respectively n_1 and n_2 branches.

Now consider the second-order correlation function: F_2^ϵ can be described by a collision graph constructed from two collision trees with roots 1^* and 2^* , and $n_1 + n_2$ branches. The main difference with $F_1^\epsilon \otimes F_1^\epsilon$ is that the particles in the 1^* and 2^* trees may interact. We can thus decompose the trees constituting F_2^ϵ into two categories: those such that there is at least one collision involving a particle from each tree (such a recollision will be called *external*), and the others (Figure 5).

Note, however, that two collision-free trees do not correspond to independent trees, precisely because of the dynamical exclusion condition. This exclusion condition can itself be decomposed as $1_{1^* \rightsquigarrow 2^*} = 1 - 1_{1^* \sim 2^*}$ (Figure 6), where $1_{1^* \sim 2^*}$ means that there is an overlap at some point between a particle from the 1^* tree and a particle from the 2^* tree. This decomposition is a pure mathematical artifact, and the $1^* \sim 2^*$ overlap condition does not affect the dynamics (the overlapping particles are not deflected).

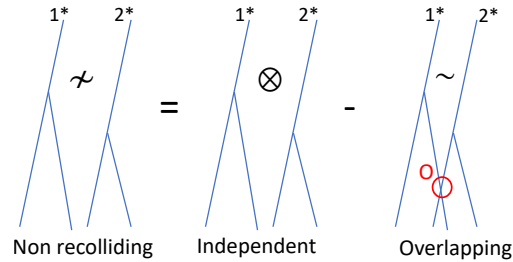


Figure 6. Decomposition of the dynamical exclusion condition.

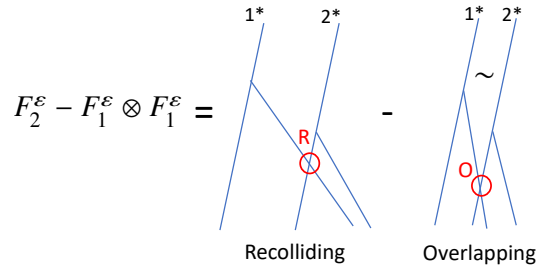


Figure 7. The second-order cumulant corresponds to the occurrence of at least one external recollision or an overlap.

Let us now define the *second-order rescaled cumulant*

$$f_2^\epsilon := \mu_\epsilon (F_2^\epsilon - F_1^\epsilon \otimes F_1^\epsilon). \quad (3.1)$$

The previous discussion indicates that this cumulant is represented by trees that are coupled by external collisions or overlaps (Figure 7). In view of definition (3.1) and the discussion in Section 2.3 giving an $O(t/\mu_\epsilon)$ estimate of the Lebesgue measure of configurations giving rise to a collision, one can expect f_2^ϵ to be uniformly bounded in L^1 and therefore to have a limit f_2 in the sense of the measures. One can prove in addition that f_2 corresponds to trees with *exactly* one external recollision or overlap on $[0, t]$: any other interaction between the trees gives rise to additional smallness and is therefore negligible.

Remark 3.1. The initial measure does not factorize exactly ($F_2^{\varepsilon,0} \neq F_1^{\varepsilon,0} \otimes F_1^{\varepsilon,0}$) because of the static exclusion condition. Thus, the initial data also induce a small contribution to f_2^ε , but this contribution is significantly smaller than the dynamical correlations (by a factor ε).

3.2 The cumulant generating function

For a Gaussian process, the first two correlation functions F_1^ε and F_2^ε determine completely all other k -particle correlation functions F_k^ε , but in general, part of the information is encoded in the cumulants of higher order ($k \geq 3$)

$$f_k^\varepsilon(t, Z_k) := \mu_\varepsilon^{k-1} \sum_{\ell=1}^k \sum_{\sigma \in \mathcal{P}_k^\ell} (-1)^{\ell-1} (\ell-1)! \prod_{i=1}^{\ell} F_{|\sigma_i|}^\varepsilon(t, Z_{\sigma_i}),$$

where \mathcal{P}_k^ℓ is the set of partitions of $\{1, \dots, k\}$ into ℓ parts with $\sigma = \{\sigma_1, \dots, \sigma_\ell\}$, $|\sigma_i|$ being the cardinality of the set σ_i and $Z_{\sigma_i} = (z_j)_{j \in \sigma_i}$. Each cumulant encodes finer and finer correlations. Contrary to the correlation functions (F_k^ε), the cumulants (f_k^ε) do not duplicate the information which is already encoded at lower orders. From a geometric point of view, we can extend the analysis of the previous section and show that the cumulant f_k^ε of order k can be represented by k trees that are completely connected either by external collisions, or by overlaps (Figure 8). These dynamical correlations can be classified by a signed graph with k vertices representing the different trees, coding tree collisions (the corresponding edges take a + sign) and overlaps (the corresponding edges take a - sign). We can then systematically extract a minimally connected graph T by identifying $k-1$ "aggregations" of tree collisions or overlaps. We then expect f_k^ε to decompose into a sum of $2^{k-1} k^{k-2}$ terms, where the factor k^{k-2} is the number of trees with k numbered vertices (from Cayley's formula). For each given signed minimally connected graph, the collision/overlap conditions correspond to $k-1$ independent constraints on the configuration z_1^*, \dots, z_k^* at time t . Therefore, neglecting the issue of large velocities, this contribution to the cumulant f_k^ε has a Lebesgue measure of size $O((t/\mu_\varepsilon)^{k-1})$, and we derive the estimate

$$\|f_k^\varepsilon\|_{L^1} \leq \mu_\varepsilon^{k-1} C^k \times 2^{k-1} k^{k-2} \times (t/\mu_\varepsilon)^{k-1} \leq k! C(Ct)^{k-1}. \quad (3.2)$$

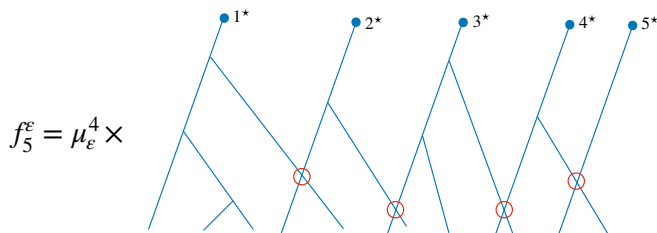


Figure 8. The cumulant of order k corresponds to trees with roots in $1^*, \dots, k^*$ that are completely connected by external collisions or overlaps.

A geometric argument similar to the one developed in Lanford's proof and recalled in the analysis of the second-order cumulant above shows that f_k^ε converges to a limiting cumulant f_k and that only graphs with exactly $k-1$ external collisions or overlaps (and no cycles) contribute in the limit.

Note further that a classical and rather simple calculation (based on the series expansions of the exponential and logarithm) shows that the cumulants are nothing but the coefficients of the series expansion of the exponential moment:

$$\begin{aligned} \mathcal{I}_t^\varepsilon(h) &:= \frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon[\exp(\mu_\varepsilon \langle \pi_t^\varepsilon, h \rangle)] \\ &= \sum_{k=1}^{\infty} \frac{1}{k!} \int f_k^\varepsilon(t, Z_k) \prod_{i=1}^k (e^{h(z_i)} - 1) dZ_k. \end{aligned} \quad (3.3)$$

The quantity $\mathcal{I}_t^\varepsilon(h)$ is called the *cumulant generating function*. Estimate (3.2) provides the analyticity of $\mathcal{I}_t^\varepsilon(h)$ in short time as a function of e^h , and this uniformly with respect to ε (sufficiently small). The limit \mathcal{I}_t of $\mathcal{I}_t^\varepsilon$ can then be determined as a series in terms of the limiting cumulants f_k ,

$$\mathcal{I}_t(h) = \sum_{k=1}^{\infty} \frac{1}{k!} \int f_k(t, Z_k) \prod_{i=1}^k (e^{h(z_i)} - 1) dZ_k.$$

In a suitable functional setting [5], it can be shown that this functional satisfies a Hamilton–Jacobi equation

$$\partial_t \mathcal{I}_t(h) = \int dz \frac{\partial \mathcal{I}_t(h)}{\partial h} v \cdot \nabla_x h + \mathcal{H} \left(\frac{\partial \mathcal{I}_t(h)}{\partial h}, h \right)$$

with initial condition $\mathcal{I}(0, h) = \int dz f^0(e^h - 1)$ and Hamiltonian \mathcal{H} given by

$$\mathcal{H}(\varphi, h) := \frac{1}{2} \int \varphi(z_1) \varphi(z_2) (e^{\Delta h} - 1) d\mu(z_1, z_2, \omega), \quad (3.4)$$

where $\Delta h(z_1, z_2, \omega) = h(z_1') + h(z_2') - h(z_1) - h(z_2)$. We use here notation (2.2) for the pre-collisional velocities and the definition

$$d\mu(z_1, z_2, \omega) := \delta_{x_1-x_2}((v_1 - v_2) \cdot \omega)_+ d\omega dv_1 dv_2 dx_1.$$

The successive derivatives of this functional being precisely the limit cumulants f_k , the successive derivatives of the Hamilton–Jacobi equation provide the evolution equations of these cumulants: for example, differentiating this equation once produces the Boltzmann equation, differentiating it twice produces the equation of the covariance described in the next paragraph.

3.3 Fluctuations

The control of the cumulant generating function allows in particular to obtain the convergence of the fluctuation field defined in (1.4) and thus to analyze the dynamical fluctuations over a time T^* of the same order of magnitude as the convergence time T_L of Theorem 2.1.

Theorem 3.2 (Bodineau, Gallagher, Saint-Raymond, Simonella [5]). *The fluctuation field ζ_t^ε converges, in the low density limit and on a time interval $[0, T^*]$, towards a process ζ_t , solution to the fluctuating Boltzmann equation*

$$\begin{cases} d\zeta_t = \underbrace{\mathcal{L}_t \zeta_t dt}_{\text{linearized Boltzmann operator}} + \underbrace{d\eta_t}_{\text{Gaussian noise}}, \\ \mathcal{L}_t h = \underbrace{-v \cdot \nabla_x h}_{\text{transport}} + \underbrace{C(f_t, h) + C(h, f_t)}_{\text{linearized collision operator}}, \end{cases} \quad (3.5)$$

where f_t is the solution at time t to the Boltzmann equation (2.1) with initial data f^0 , and $d\eta_t$ is a centered Gaussian noise delta-correlated in t, x with covariance

$$\text{Cov}_t(h_1, h_2) = \frac{1}{2} \int dz_1 dz_2 d\omega ((v_2 - v_1) \cdot \omega)_+ \delta_{x_2 - x_1} f(t, z_1) f(t, z_2) \Delta h_1 \Delta h_2(z_1, z_2, \omega),$$

where $\Delta h(z_1, z_2, \omega) = h(z'_1) + h(z'_2) - h(z_1) - h(z_2)$.

The limiting process (3.5) was conjectured by Spohn in [25], and this reference also presents a large panorama on the theory of fluctuations in physics. In the context of dynamics with random collisions, a similar result is shown by Rezakhanlou in [24]. In the deterministic setting, the noise obtained in the limit is a consequence of the asymptotically unstable structure of the microscopic dynamics (Figure 2) combined with the randomness of the initial data at small scales.

3.4 Large deviations

The strength of the cumulant generating function becomes really apparent at the level of large deviations, i.e., for very improbable trajectories that are at a “distance” $O(1)$ from the averaged dynamics: roughly speaking, we can show that the probability of observing an empirical distribution close to the density $\varphi(t, x, v)$ during the time interval $[0, T]$ decays exponentially fast with a rate quantified by a functional $\mathcal{F}_{[0, T]}$ which evaluates the cost of this deviation in the low density asymptotics

$$\mathbb{P}_\varepsilon(\pi_t^\varepsilon \approx \varphi_t, \forall t \leq T) \sim \exp(-\mu_\varepsilon \mathcal{F}_{[0, T]}(\varphi)). \quad (3.6)$$

The proximity between π^ε and φ is measured in the weak topology on the Skorokhod space of measure-valued functions. A precise formulation of (3.6) and a proof can be found in [6]. The result of [6] can be summarized as follows: for a class of functions φ in a neighborhood of the solution to the Boltzmann equation, there exists a time interval $[0, T^*]$ where the asymptotic (3.6) is characterized by a functional $\mathcal{F}_{[0, T^*]}$ obtained by a certain Legendre transform of the Hamiltonian \mathcal{H} defined by (3.4). This functional is identical to the one conjectured in [9, 24], by analogy with stochastic collision models of Kac type [2, 15, 18, 23]. Let us also note that the limiting SPDE (3.5) could be predicted by the same analogy

with Kac’s model for which collisions are modeled by a Markov process [19, 20]. Thus, the statistical analysis of the fluctuations and large deviations of the empirical measure confirms the robustness of Boltzmann’s intuition (cf. Section 2.1): even on exponentially small scales, the behavior of the empirical measure of a hard sphere gas is identical to that of a model of particles with random collisions depending only on the local density. This does not contradict the Hamiltonian structure of the microscopic dynamics. Memory effects persist, but they are encoded in ways that are “transverse” to the empirical measure (or at different spatial scales).

4 Conclusion

Over a short time, Lanford’s theorem states the convergence of the empirical measure of a hard sphere gas to the solution to the Boltzmann equation (Theorem 2.1). This result is completed by the analysis of fluctuations (Theorem 3.2) and large deviations (Section 3.4) of the empirical measure. These stochastic corrections are proved on times of the same order of magnitude as Lanford’s theorem.

The strategy of the proof consists in tracking how the randomness of the initial measure is transported by the dynamics of hard spheres and how the instability of this dynamics transfers, in the low density asymptotics, the initial randomness into a dynamical white noise (space/time). The convergence time is limited because the current proof gives only rough estimates of the dynamical correlations, obtained by considering that collisions only destroy the initial chaos by forming larger and larger aggregates of correlated particles. An important step to progress in the mathematical understanding of these models would be to show that the disorder is not simply the result of the initial data, but that it can be regenerated by the mixing properties of the dynamics.

A more favorable framework for controlling long time evolution is to consider an initial measure obtained as a perturbation of an equilibrium measure. The stationarity of the equilibrium measure then becomes a key tool to control dynamical correlations. The simplest case consists in perturbing only one particle, which shall be called the tagged particle, and to study its evolution over time. In [3], it is established that this particle follows a Brownian motion for large times. Another case where we know how to use the invariant measure is the study of the fluctuation field at equilibrium. In a series of recent works [5, 7], Theorem 3.2 has been generalized to arbitrarily large, and even slightly divergent, kinetic times. This allows in particular to derive the fluctuating hydrodynamic Stokes–Fourier equations.

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