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► **To cite this version:**

Vincent Ardourel. Irreversibility in the derivation of the Boltzmann equation. Foundations of Physics, 2017, 47 (4), pp.471-489. hal-01918274

HAL Id: hal-01918274

<https://hal.science/hal-01918274>

Submitted on 10 Nov 2018

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Irreversibility in the derivation of the Boltzmann equation

Vincent Ardourel

Received: date / Accepted: date

Abstract Uffink and Valente (2015) claim that there is no time-asymmetric ingredient that, added to the Hamiltonian equations of motion, allows to obtain the Boltzmann equation within the Lanford’s derivation. This paper is a discussion and a reply to that analysis. More specifically, I focus on two mathematical tools used in this derivation, viz. the Boltzmann-Grad limit and the incoming configurations. Although none of them are time-asymmetric ingredients, by themselves, I claim that the use of incoming configurations, as taken within the Boltzmann-Grad limit, is such a time-asymmetric ingredient. Accordingly, this leads to reconsider a kind of *Stoßzahlansatz* within Lanford’s derivation.

Keywords Boltzmann equation · Lanford’s theorem · Boltzmann-Grad limit · irreversibility · time-reversal invariance · *Stoßzahlansatz*

1 Introduction

The derivation of the Boltzmann equation (BE) from the Hamiltonian equations of motion of a hard spheres gas is a key topic on irreversibility (Sklar 1993, p. 32, Uffink 2007, Section 4). Although the Hamiltonian equations of motion are invariant under time reversal, the BE is not. Moreover, this equation allows to derive the H -theorem, which states that a function H monotonically decreases with time, and thus that the minus- H function increases, in agreement with the second law of thermodynamics. The derivation of the BE thus raises the question of irreversibility since this equation exhibits irreversibility even though the microscopic description of the gas is based on reversible equations.

Recent discussions (Valente 2014, Uffink and Valente 2015) focus on a rigorous derivation of the BE provided by Lanford (1975, 1976), which is “maybe

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the most important mathematical result of kinetic theory” (Villani 2010, p. 100). This result is very important from a philosophical point of view since the BE is derived without the famous controversial Boltzmann’s assumption, i.e., the *Stosszahlansatz* (Uffink and Valente 2015, p. 407 and p. 423).¹ Nevertheless, the origin of irreversibility in this derivation is still unclear and controversial. Uffink and Valente conclude their detailed analysis as follows:

We discussed the problem of the emergence of irreversibility in Lanford’s theorem. We argued that all the different views on the issue presented in the literature miss the target, in that they fail to identify a time-asymmetric ingredient that, added to the Hamiltonian equations of motion, would obtain the Boltzmann equation. More to the point, we argued that there is no such an ingredient at all, as one can infer from the fact that the theorem is indeed time-reversal invariant. (Uffink and Valente 2015, p. 432)

According to Uffink and Valente, Lanford’s theorem does not account for the appearance of irreversibility within the BE. This paper aims at replying to that analysis. More precisely, I focus on two views of the literature on the derivation BE, which are the role of the Boltzmann-Grad (B-G) limit and the role of the incoming configurations. Uffink and Valente (2015) claim that neither the B-G limit, nor the incoming configurations are time-asymmetric ingredients that allow to obtain the BE. Although I agree that none of them are a time-asymmetric ingredient, by themselves, I claim that the use of incoming configurations, as taken within the B-G limit, is such a time-asymmetric ingredient.

The paper is organized as follows. First, I introduce the derivation of the BE within Lanford’s and successors’ works, and I make clear how the question of irreversibility is tackled within this derivation (Section 2). Then, I examine why the B-G limit as well as the incoming configurations are essential to derive the BE although each of them, taken separately, is not sufficient for the appearance of irreversibility. For that purpose, I begin with the case of the B-G limit (Section 3), and then I turn to the case of the incoming configurations (Section 4). After having clarified these points, I argue that the incoming configurations *as taken within* the B-G limit are a time-asymmetric ingredient that allows to obtain the BE (Section 5). Finally, I suggest that such an analysis of Lanford’s derivation of the BE allows us to argue for a reconsideration of the *Stoßzahlansatz* of the original Boltzmann’s heuristic derivation of the BE (Section 6).

¹ In Boltzmann’s derivation, *Stoßzahlansatz*, sometimes wrongly called the hypothesis of molecular chaos as Uffink and Valente point out, was assumed at any time. With Lanford’s derivation, there is only a factorization condition at the initial time. See Section 2.2 and Section 6 of the paper.

2 The derivation of the Boltzmann equation

The BE is based on a model of a hard spheres gas. It describes the time evolution of the probability density that a hard sphere is located at the position q with the momentum p . The original Boltzmann's derivation of the equation and the H -theorem led to extended discussions that cannot be addressed here (Uffink 2007, Brown et al. 2009). Yet based on Grad's ideas (1949), Lanford (1975, 1976) provided a rigorous derivation, with some gaps, which have been completed by Cercignani et al. (1994) and Gallagher et al. (2014). The aim of this section is to give an overview of the main steps of this rigorous derivation of the BE.² I begin by introducing the BE (Section 2.1) before sketching the main steps of its derivation (Section 2.2). I then introduce the question of irreversibility within Lanford's derivation of the BE (Section 2.3).

2.1 The Boltzmann equation and the H -theorem

Let us consider a model of N hard spheres with mass m and diameter a that move freely according to the laws of classical dynamics. Let us denote by q and p , the position and the momentum of the center of the mass of a hard sphere in three dimension space. Under these conditions, two spheres i and j collide when the relative position between the center of the spheres $|q_i - q_j| = a$. In this case, with $p_{i,j}$ the momenta before collision, the momenta after collision $p'_{i,j}$ are given by:

$$p'_i = p_i - (\omega_{ij} \cdot (p_i - p_j)) \omega_{ij} \quad (1)$$

$$p'_j = p_j + (\omega_{ij} \cdot (p_i - p_j)) \omega_{ij} \quad (2)$$

with ω_{ij} is the unit vector $\omega_{ij} = \frac{q_j - q_i}{a}$.³

Let us now describe the gas by a function $f_t(q, p_1)$ that represents the probability density that the particle 1 is located at the position between q and $q + dq$ with momenta between p_1 and $p_1 + dp_1$ at the instant t . Under these conditions, the BE is:

$$\frac{\partial}{\partial t} f_t(q, p_1) + \frac{p_1}{m} \cdot \frac{\partial}{\partial q} f_t(q, p_1) = \mathcal{Q} \quad (3)$$

with \mathcal{Q} the collision term defined as:

$$\mathcal{Q} = \alpha \int_{\mathbf{R}^3} dp_2 \int_{\mathbf{S}_+} d\omega_{12} \frac{(p_1 - p_2)}{m} \cdot \omega_{12} \{f_t(q, p'_1) f_t(q, p'_2) - f_t(q, p_1) f_t(q, p_2)\} \quad (4)$$

² This section is a summary based on Uffink and Valente (2015) and Cercignani et al. (1994, Chapter 4). For technical details, see also Gallagher et al. (2014) and Golse (2013).

³ I follow the notation used by Uffink and Valente (2015) and Golse (2014, p. 3). I emphasize that, in Gallagher (2014, p. 5), ω_{ij} is instead defined as $\frac{q_i - q_j}{a}$, from the particule i to the particule j .

where \mathbf{S}_+ is the domain for ω_{12} such as $\omega_{12} \cdot (p_1 - p_2) \geq 0$. This corresponds to the case for which particles are about to collide.⁴

The BE allows then to derive the H -theorem. Let us first define the H -function, which is more precisely a functional, as follows:

$$H(f_t) = \int f_t(q, p) \ln f_t(q, p) dp dq \quad (5)$$

In a nutshell, it can be proved that $\frac{dH(f_t)}{dt} \leq 0$, i.e., the H -function monotonically decreases with time. The BE thus exhibits irreversibility in the sense that the minus H -function, which increases with time, can be somehow interpreted as the entropy of the system.

2.2 Main steps of the derivation

Let us turn to the Lanford's derivation of the BE, which requires different main steps that I sketch very briefly.

Step 1: From the Liouville equation to the BBGKY hierarchy

The derivation of BE begins with the Liouville equation of a N hard spheres system that describes the time evolution of the probability density $\mu(x_1, x_2, \dots, x_N)$ in the phase space:

$$\frac{\partial \mu}{\partial t} = \{H, \mu\} = \sum_{i=1}^{3N} \frac{\partial H}{\partial q_i} \frac{\partial \mu}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial \mu}{\partial q_i} =: \mathcal{H}_N \mu \quad (6)$$

where H is the Hamiltonian of the system. Using the property that the Hamiltonian is invariant by permutation of particles, and under some normalization conventions, a hierarchy of marginal probability densities (or reduced probability densities) is defined as follows:

$$\begin{aligned} \rho_1(x_1) &:= \int \mu(x_1, \dots, x_N) dx_2 \cdots x_N \\ &\vdots \\ \rho_k(x_1, \dots, x_k) &:= \int \mu(x_1, \dots, x_N) dx_{k+1} \cdots x_N \\ &\vdots \\ \rho_N(x_1, \dots, x_N) &:= \mu(x_1, \dots, x_N) \end{aligned}$$

⁴ Indeed, two particles 1 and 2 are about to collide if their relative distance ω_{12} decreases with time, i.e., if $\frac{d}{dt} |q_2 - q_1|^2 \leq 0$, which implies that $\omega_{12} \cdot (p_1 - p_2) \geq 0$ with our notations.

where $\rho_k(x_1, \dots, x_k)$ corresponds to the probability density that k particles are located at q_1, \dots, q_k and with momenta p_1, \dots, p_k , while the remaining $N - k$ particles possess arbitrary positions and momenta.

Then, applying the Liouville equation to the ρ_k , one obtains the BBGKY hierarchy, i.e., a series of N equations:

$$\frac{\partial \rho_{k,t}}{\partial t} = \mathcal{H}_k \rho_{k,t} + \mathcal{C}_{k,k+1}^{(a)} \rho_{k+1,t} \quad k \in \{1, \dots, N\} \quad (7)$$

with

$$\mathcal{C}_{k,k+1}^{(a)} \rho_{k+1,t} = Na^2 \sum_{i=1}^k \int_{R^3} dp_{k+1} \int_{S^2} d\omega_{i,k+1} \quad (8)$$

$$(\omega_{i,k+1} \cdot (p_{k+1} - p_i)) \rho_{k+1,t}(x_1, \dots, x_k, q_i + a\omega_{i,k+1}, p_{k+1}) \quad (9)$$

Step 2: From the BBGKY hierarchy to the Boltzmann hierarchy

The integral in the collision term $\mathcal{C}_{k,k+1}^{(a)}$ is then split into two terms and the B-G limit is used. Under these conditions, one proves that the BBGKY hierarchy tends formally to the Boltzmann hierarchy:

$$\frac{\partial f_{k,t}}{\partial t} = \mathcal{H}_k f_{k,t} + \mathcal{C}_{k,k+1} f_{k+1,t} \quad (10)$$

with $\mathcal{C}_{k,k+1}^{(a)} \rightarrow \mathcal{C}_{k,k+1}$, $\rho_{k,t} \rightarrow f_{k,t}$, $Na^2 \rightarrow \alpha$, where

$$\mathcal{C}_{k,k+1} f_{k+1,t} = \quad (11)$$

$$\alpha \sum_{i=1}^k \int_{R^3} dp_{k+1} \int_{\omega_{i,k+1} \cdot (p_i - p_{k+1}) \geq 0} d\omega_{i,k+1} (\omega_{i,k+1} \cdot (p_i - p_{k+1})) \quad (12)$$

$$[f_{k+1,t}(x_1, \dots, q_i, p_i', \dots, q_i, p_{k+1}') - f_{k+1,t}(x_1, \dots, q_i, p_i, \dots, q_i, p_{k+1})] \quad (13)$$

Step 3: From the Boltzmann hierarchy to the Boltzmann equation

Finally, let us consider a specific solution for the Boltzmann hierarchy, which is the factorized solution :

$$f_{k,t}(x_1, \dots, x_k) = \prod_{i=1}^k f_t(x_i) \quad (14)$$

where $f_t(x_i)$ is the solution of the BE. In this case, the equations of the Boltzmann hierarchy correspond to the BE. Moreover, if we add the further assumption about the initial conditions for the distribution, namely that is the functions $f_{k,0}$ factorize in such a way that:

$$f_{k,0}(x_1, \dots, x_k) = \prod_{i=1}^k f_0(x_i), \quad (15)$$

then it can be shown that this factorization property (Eq. 14) is maintained in time, which is called the *propagation of chaos*.

2.3 The question of irreversibility within Lanford's theorem

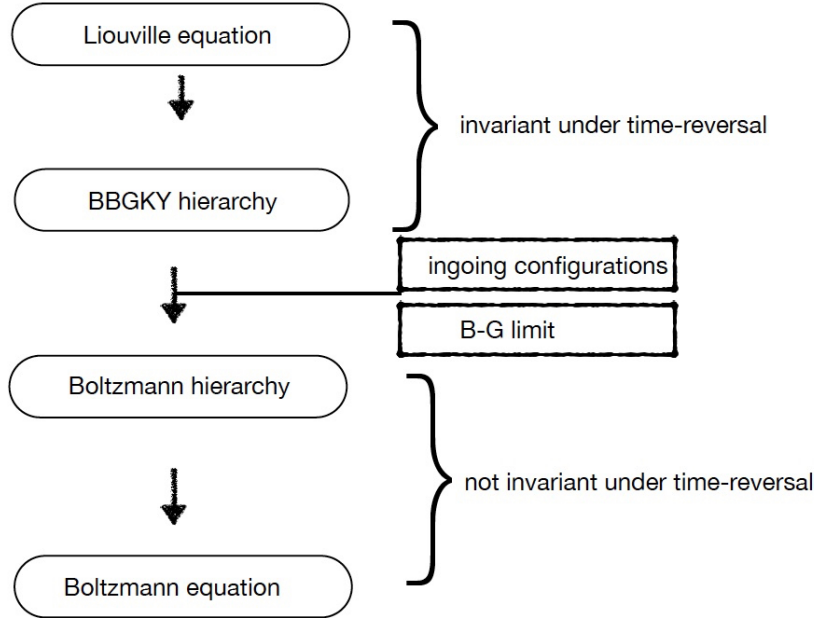


Fig. 1 Main steps of Lanford's derivation of the Boltzmann equation.

The step 2 of the derivation is particularly important with regard to the question of irreversibility. As Lanford points out, “the BBGKY hierarchy is time-reversal invariant but the Boltzmann hierarchy is not” (Lanford 1975, p. 110). Like the Liouville equation, the BBGKY hierarchy is indeed invariant under time reversal. Instead, the Boltzmann hierarchy, like the BE, is not invariant under time reversal. Irreversibility thus seems to appear between the BBGKY hierarchy and the Boltzmann hierarchy.

Two ingredients are required within this second step, which are the B-G limit and the ingoing (or incoming) configurations (see Fig. 1). First, the B-G limit is the limiting regime for which the number N of hard spheres tends to infinity, the diameter a of spheres tends to zero in such a way that the quantity Na^2 converges to a finite and non-zero quantity α (Grad 1949). It is a limit for infinitely diluted gases since the volume occupied by bodies, which varies with Na^3 , tends to zero. As Uffink and Valente (2015) point out, “since irreversible

behaviour already appears at the level of the Boltzmann hierarchy, Lanford puts the blame on the procedure to take the limit from the BBGKY hierarchy to the Boltzmann hierarchy” (p. 423). Second, the ingoing configurations are the momenta, or the velocities, of two hard spheres *before* colliding (Fig. 2). They are also called pre-collisional configurations and are used to rewrite the collision term $C_{k,k+1}^{(a)}$ of the BBGKY hierarchy in order to obtain the collision term $C_{k,k+1}$ of the Boltzmann hierarchy. Such configurations contrast with outgoing configurations, which are the momenta *after* collision, also called post-collisional configurations. However, because the collisions between two hard spheres are deterministic (see Eq. (1)-(2)), the use of the one or the other configuration seems to be equivalent.

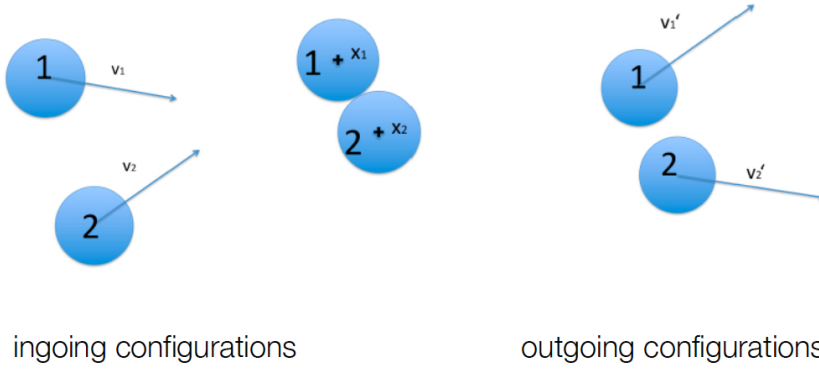


Fig. 2 Ingoing and outgoing configurations. Figure extracted from (Saint-Raymond 2013).

Uffink and Valente (2015) claim that neither the B-G limit, nor the ingoing configurations are responsible for the appearance of irreversibility. Their arguments are specific for each of them, and they will be discussed in the remainder of the paper. But, before investigating them, I make clear another and more general claim they argue for: *there is no time-asymmetric ingredient at all since Lanford’s theorem is time-reversal invariant*. Uffink and Valente (2015, p. 431) indeed emphasize that the theorem is valid not only for positive times but also for negative times, i.e., valid within a interval $[-\tau, \tau]$. Lanford (1975, p. 109) himself stressed this point. Although the BE is derived for positive times, another equation is indeed derived for negative times within Lanford’s theorem, which is the anti-BE (or the backward BE):

$$\frac{\partial}{\partial t} f_t(q, p_1) + \frac{p_1}{m} \cdot \frac{\partial}{\partial q} f_t(q, p_1) = \mathcal{Q}^* \quad (16)$$

with \mathcal{Q}^* the collision term that is the opposite of the collision term in the BE, i.e., $\mathcal{Q}^* = -\mathcal{Q}$. The anti-BE is an equation that is also non invariant under time reversal. However, this equation is problematic with regard to the

question of the appearance of irreversibility because it leads to an anti- H theorem, which states that, for negative times, the H function increases with time, or the minus H function decreases with time (Fig. 3). This seems to be in conflict with the the second law of thermodynamics which states that entropy is monotonic for any times. Therefore, as Valente (2014, p. 326) stresses, this property raises the question whether Lanford's theorem is true for the past.

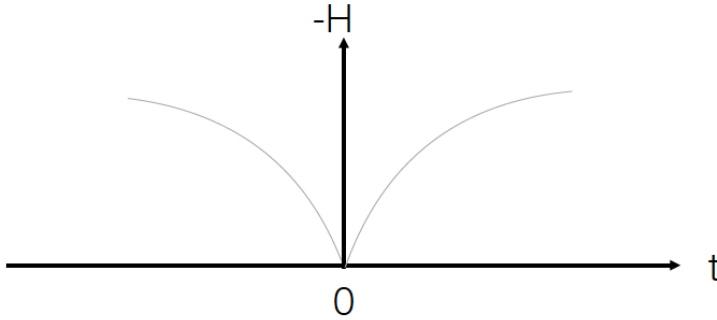


Fig. 3 Time-symmetry of H -theorem derived from Lanford's theorem.

Lanford's theorem is time-symmetric in the sense that it is valid within a interval $[-\tau, \tau]$. However, I claim that it does not follow that there is no time-asymmetric ingredient used to derive the BE from the Hamiltonian equations of motion within Lanford's and successors' derivation. As I will argue in Section 5, the use of the ingoing configurations to represent collisions between particles forces the derivation of the BE rather than the anti-BE. One should thus make the distinction between the Lanford's theorem and the Lanford's derivation of the BE. Lanford's theorem can be applied to both ingoing and outgoing configurations. In the first case, it leads to the BE for the positive times (for $[0, \tau)$) and, in the second case, to the anti-BE for the negative times (for $[-\tau, 0]$). Accordingly, I will argue in Section 5 that ingoing configurations, as taken within the B-G limit, are the time-asymmetric ingredient that allows to derive the BE from Hamiltonian equation of motions. But before that, I investigate the role of the B-G limit within Lanford's derivation (Section 3), and then, the role the incoming configurations (Section 4).

3 The Boltzmann-Grad limit: essential for the derivation but not sufficient for irreversibility

In this section, I make clear why the B-G limit is essential for the derivation of the BE although it is not sufficient for the appearance of irreversibility. This section is a first step before arguing below, in Section 5, in what sense the

B-G limit nevertheless contributes to the appearance of irreversibility within Lanford's derivation.

3.1 The essential role the Boltzmann-Grad limit in the derivation

Valente (2014) and Uffink and Valente (2015) make clear that the B-G limit is essential in the derivation of the BE:

[W]e would like to stress that the Boltzmann-Grad limit is essential for the purpose of obtaining a rigorous derivation of the Boltzmann equation, from which one derives a statistical H -theorem predicting a monotonic increase of entropy towards equilibrium. (Valente 2014, p. 321)

This limiting procedure first enables to rigorously establish the relationship between the microstate of the gas and the probability density of the gas at the macroscopic scale. At the microscopic scale, the distribution function of the gas of hard spheres involves a discrete system, i.e., composed by finite number N of hard spheres located at positions q_i with momenta p_i , with $i = 1, \dots, N$. By contrast, the probability density $f_t(x_i)$ of the BE is a continuous function of the variables q and p . The B-G scaling thus offers a rigorous framework to approximate a discrete distribution by a continuous function by using the limit for which the number of components tends to infinity.⁵ Second, the use of the B-G scaling guarantees that the collision term in the BE does not vanish when the diameter a of hard spheres then to zero. This scaling maintains indeed the quantity Na^2 to be finite, which corresponds to the factor α of the collision integral of the BE.⁶

Besides, it has to be stressed that the derivation of the BE is not doomed to use a hard sphere model. More generally, this derivation requires a *strong but local* coupling between particles. This can be exemplify by a hard sphere

⁵ The use of the B-G limit avoids thus to meet the recurrence objection since the recurrence theorem rests on the assumption that N is finite (Jones 2006, p. 105) and Valente (2014, p. 321).

⁶ Norton (2012, p. 218) points out that extensionless points with the B-G limit are problematic with respect to determinism. When $a \rightarrow 0$ the direction of particles after each collision is no longer deterministic. Valente (2014, p. 320) reinforces this point in emphasizing that the vector ω_{12} corresponding to the relative position of the centers of two hard spheres that are going to collide is no more defined when $a \rightarrow 0$. In addition, Golse (2014, p. 35) suggests that the appearance of irreversibility could thus be linked with such appearance of indeterminism:

Another factor that contributes to the irreversibility is that B-G limit implies that $r \rightarrow 0$ [i.e. $a \rightarrow 0$]. While $r > 0$, laws of collisions are reversible because there is a unique vector n_{kl} [i.e. ω_{12}] with respect to the position of particles k and l [i.e. 1 and 2]. Instead, when $r \rightarrow 0$, the definition of the collision integral [...] requires the vector n , analogous to n_{kl} , which is now randomly and uniformly distributed on the sphere.⁷

However, the relationship, if there is any, between the appearance of indeterminism in the laws of collision and the loss of invariance under time-reversal for the BBGKY hierarchy is still not clear.

model but, also by a model of N mass points where two mass points interact with a short-range repulsive potential (King 1975, Gallagher et al. 2014). Such a derivation of the BE still requires the B-G limit for which a is now the range of a short-range repulsive potential. In that case, the B-G limit allows to make compatible the use of an infinite limit for Hamiltonian systems with the constraint that average energy per particle remains bounded. This is done by assuming that the energy of each pairwise interaction is small, which is done “by scaling the range of potential” (Gallagher et al. 2014, p. 7).

Although the B-G limit is essential for the derivation of the BE, I stress that it is not a time-asymmetric ingredient in the derivation of the BE, in agreement with Uffink and Valente’s claim (2015). In the remainder of this Section 3, I untangle the reasons of why the B-G limit is not sufficient for the appearance of irreversibility.

3.2 Boltzmann-Grad limit and the Vlasov equation

About the B-G limit, Uffink and Valente emphasize that “Lanford (1981) himself argues that *this* limiting procedure is not sufficient for the appearance of irreversibility.” (2015, p. 424. My emphasis). Following a comparison made by Lanford between the derivation of the BE and the derivation of the Vlasov equation, they argue that the B-G limit is not a time-asymmetric ingredient in the derivation of the BE. Indeed, the two equations are actually very different with regard to the question of irreversibility. On the one hand, the VE is time-reversal invariant whereas the BE is not. On the other hand, the H -function for the VE, occurring in the H -theorem, is constant with time whereas the H -function for the BE monotonically decreases with time. However, I stress here that this comparison is misleading to argue that the B-G limit is not sufficient for the appearance of irreversibility.⁸

Unlike the BE, the derivation of the VE does not actually require the B-G limit. It requires the *effective field* or the *mean field limit*, which only assume that $N \rightarrow \infty$ in order to scale the strength of interactions. There is not any a parameter within this limiting regime. The derivations of the BE and the VE are indeed based on two different limiting regimes. Unlike the BE, the derivation of the VE assumes a *weak but global* coupling between particles, which is a model where each particle interacts with other particles without colliding (Gallagher et al. 2014, p. 7). Coupling is weak in the sense that the strength of the individual interaction becomes small when N grows (since potential varies with $1/N$). However, the range of the potential remains

⁸ The VE describes the evolution of the probability density in phase-space that a particle is located at the position q with momentum p when the interaction between particles is given by a sum of two-body potentials of the form : $\phi^{(N)}(q_1 - q_2) = \frac{1}{N} \phi_0(q_1 - q_2)$. The BE and the VE thus both describe the evolution of the probability density $f_t(q, p)$ of a N -body system. The VE is : $\frac{\partial}{\partial t} f_t(q, p) + \frac{p}{m} \cdot \frac{\partial}{\partial q} f_t(q, p) = -\mathcal{F}(q) \frac{\partial}{\partial p} f_t(q, p)$ where $\mathcal{F}(q)$ is an integral that depends on the potential ϕ_0 and $f_t(q, p)$ (Lanford 1981, p. 75). In addition, both equations are derived from the Hamiltonian equations of motion of N particles when the number of particles tends to infinity.

macroscopic in the sense that two particles which are far from each other still interact with each other.⁹

Like the B-G limit, the effective field limit, allows to make compatible the use of an infinite limit for Hamiltonian systems with the constraint that average energy per particle remains bounded. However, in this case, this is done by assuming that the energy of each pairwise interaction is small “by scaling the strength of the force” (Gallagher et al. 2014, p. 7). Since the derivation of the VE does *not* require the B-G limit, I stress that we are not allowed to make any statements about the B-G limit from the analysis of the VE.

3.3 Boltzmann-Grad limit and time-symmetry of Lanford’s theorem

A most compelling reason for arguing that the B-G limit is not sufficient for the appearance of irreversibility comes from the time-symmetry of Lanford’s theorem, which is stressed by Uffink (2007, p. 116) and Valente (2014) (see Fig. 3):

[T]here exists a version of the theorem for negative times which provides a rigorous derivation of the Anti-Boltzmann equation (cfr. Lanford 1975 and Lebowitz 1981) [...] [This] now means that in the *Boltzmann-Grad limit* the vast majority of microstates x_0 satisfying the initial conditions evolve in agreement with Anti-B.E., from which it follows that the negative of the H -function monotonically decreases for $t < 0$ (Valente 2014, p. 328, My emphasis)

We have seen in Section 3.1 that the B-G limit is required to derive the Boltzmann hierarchy for positive times. It turns out that the B-G limit is also required to derive the anti-Boltzmann hierarchy for negative times. The analysis discussed in Section 3.1 equally applies to the anti-BE for negative times. This means that, by itself, the use of the B-G limit is essential to obtain the BE as well as the backward-BE. If the B-G limit were, by itself, a time-asymmetric ingredient within the derivation of the BE, only the BE could be derive. But, this not the case. An anti-BE is derived within the B-G limit. This means that the B-G is not a time-asymmetric ingredient in the derivation of the BE.

4 Incoming configurations: essential for the derivation but not sufficient for irreversibility

Let us turn now to the incoming configurations. I make clear why they are essential to the derivation of the BE even if they are not sufficient for the appearance of irreversibility. This section is also a first step before arguing

⁹ Unlike the BE, the VE is indeed derived from a system of N particles that do not collide: “The Vlasov equation is the kinetic model for *collisionless* gases or plasmas” (Golse 2003, p. 2, My emphasis). In addition, the derivations of the VE and the BE require two different notions of convergence.

below, in Section 5, in what sense the incoming configurations *within* the B-G limit become, under this condition, a time-asymmetric ingredient in the derivation of the BE.

4.1 The essential role of ingoing configurations

As we have seen in Section 2.3, incoming configurations correspond to the momenta of hard spheres *before* they collide whereas outgoing configurations correspond to the momenta *after* collision. A crucial step in the derivation of the BE lie in the use of these incoming configurations. This step consists in rewriting the right-hand of the equations of the BBGKY hierarchy (Eq. 7).

The right-hand of the equations of the BBGKY hierarchy $\mathcal{C}_{k,k+1}^{(a)}$ (Eq. 8) is split in two terms that will lead, latter on in the derivation, to the gain and loss terms of the right hand of the BE, i.e the collision term \mathcal{Q} of equation (4). More precisely, the integral in (Eq. 8) is split in two integrals that range over the hemispheres $\omega_{i,k+1} \cdot (p_i - p_{k+1}) \geq 0$ and $\omega_{i,k+1} \cdot (p_i - p_{k+1}) \leq 0$. In the first hemisphere, the momenta in the configuration $(q_i, p_i; q_i + a\omega_{i,k+1}, p_{k+1})$ appear as *ingoing momenta* because of the domain of integration. The particles move closer to each other. Instead, the momenta appear as *outgoing momenta* in the second hemisphere according the domain of integration. The step in the derivation that we focus on consists in rewriting the two hemispheres with *only* incoming momenta.

Lanford and Cercignani et al. emphasize that this step is crucial in the derivation with respect to the derivation of the BE:

We obtained [the BBGKY hierarchy] by systematically writing collision phase points in their incoming representations. We could have equally well have written them in their outgoing representations; [...] we would have obtained the Boltzmann collision term with its sign reversed. It is thus essential, in order to get the Boltzmann equation, to assume [...] incoming collision points (x_1, x_2) and not [...] outgoing ones (Lanford 1975, p. 88)

And similarly:

In the derivation of the [collision] operator Q , we chose to represent collision phase points in terms of ingoing configurations. [...] We are thus compelled to ask whether the representation in terms of ingoing configurations is the right one, i.e., physically meaningful. (Cercignani et al. 1994, p. 74)

According to Lanford and Cercignani et al., if there is no such change of variables, the integral vanishes by symmetry. In addition, if we use the *outgoing configuration*, a minus sign will appear in the right hand leading, latter on the derivation, to the anti-BE. Therefore, the derivation of the BE requires the use of the incoming configurations.

4.2 Ingoing configurations as neutral temporal ingredients

Although the use of the incoming configurations is essential to derive the BE, Uffink and Valente claim that they are neutral with respect to the appearance of irreversibility in the derivation of the BE.

On the one hand, they mitigate the difference between incoming and outgoing configurations with respect to the derivation the BE:

The choice of either one of the two collision configurations does not make any difference at the level of the BBGKY hierarchy. In particular, one can derive the Boltzmann hierarchy, as well as the anti-Boltzmann hierarchy, from the BBGKY hierarchy rewritten in terms of either the incoming or the outgoing configurations without having to choose the “right” one. (Uffink and Valente 2015, p. 429)

Uffink and Valente prove indeed the equivalence between the BBGKY hierarchy with the collision term expressed by incoming momenta and the BBGKY hierarchy with the collision term expressed by outgoing momenta (2015, p. 435). In the first part of their *Proposition 3*, they establish more specifically that the BBGKY hierarchy with ingoing configurations is *equal* to the BBGKY hierarchy with outgoing configurations.

On the other hand, they emphasize why the incoming configurations cannot be a time-asymmetric ingredient. First, they show in the second part of their *Proposition 3* that the BBGKY written with outgoing configurations is time-reversal invariant. More to the point, they prove in their *Proposition 2* that the BBGKY written with incoming configurations is time-reversal invariant. If the incoming configurations were a time-asymmetric ingredient in the derivation of the BE, they could not lead to a time-reversal invariance equation.

At this point of the debate, the position of Lanford and Cercignani et al. on the one hand, and the position of Uffink and Valente seem to be in conflict. Either some of them are wrong, or what they state is, in a sense, still compatible. I argue for the second option in the next section.

5 Incoming configurations *within* Boltzmann-Grad limit

In this section, I argue that *incoming configurations, as taken within the B-G limit*, is a time-asymmetric ingredient that added to Hamiltonian equations of motion allows to obtain the BE. My argument runs as follows. First of all, it is uncontroversial that incoming configurations refer to a preferred time-direction in the sense that collisions are represented by momenta *before* collision. Yet, as I will argue below, the use of these ingoing configuration *within* the B-G limit is *mandatory* in order to obtain the BE. More to the point, by using the ingoing configurations within the B-G limit, one *cannot* derive the anti-BE for negative times. In other words, the use of incoming configurations within the B-G limit leads to a time-asymmetric *H*-function. Unlike the *H*-function discussed in Section 2.3 (see Fig. 3), the *H*-function is no longer time-symmetric

by using the incoming configuration only (see Fig. 4). If we *only* use the ingoing configurations, the BE is derived for positive times within Lanford's theorem but *nothing* can be derived for negative times. Therefore, the crucial part of my discussion is to make clear that the ingoing configurations are mandatory to obtain the BE within the B-G limit.

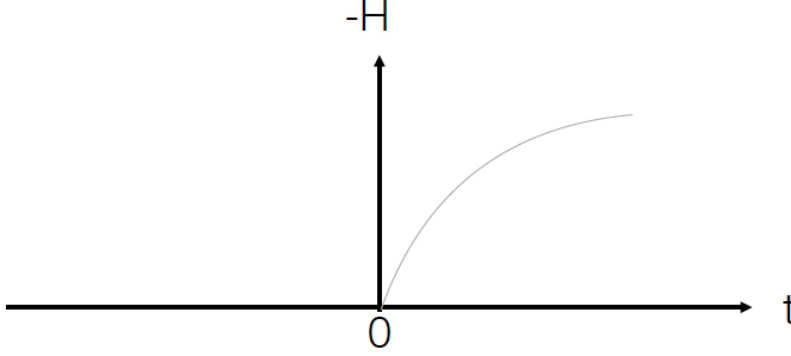


Fig. 4 H -theorem with incoming configurations and without outgoing configurations.

5.1 Express the BBGKY hierarchy vs. derive the Boltzmann hierarchy

Let us begin by focusing on the debate between Lanford (1975) and Cercignani et al. (1994), and Uffink and Valente (2015) about the incoming configurations. I argue that their positions are compatible depending on whether the B-G limit is taken or not. More precisely, I stress that the equivalence between ingoing configurations and outgoing configurations holds at the level of the BBGKY hierarchy, i.e. to *express* the BBGKY hierarchy, in agreement with Uffink and Valente: “The choice of either one of the two collision configurations does not make any difference at the level of the BBGKY hierarchy” (2015, p. 49). Nevertheless, I claim that ingoing and outgoing configurations are not equivalent to *derive* the Boltzmann hierarchy, and respectively to derive the backward Boltzmann hierarchy, which both require the B-G limit.

This claim is supported by the way that Cercignani et al. and Gallagher et al. prove that the BBGKY hierarchy converges to the Boltzmann hierarchy within the B-G limit. What is proved is that the formal solution of the BBGKY hierarchy converges to the formal solution of the Boltzmann hierarchy. On the one hand, the formal solution of the BBGKY hierarchy can be expanded as

follows:

$$\rho_k(t) = \sum_{i=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{i-1}} dt_i S_a^k(t-t_1) \mathcal{C}_{k,k+1}^{(a)} S_a^{k+1}(t_1-t_2) \cdots$$

$$\mathcal{C}_{k+i-1,k+i}^{(a)} S_a^{k+i}(t_i) \rho_{k+i}(0)$$

where $S_a(\cdot)$ are operators that represent the collisionless time evolution of the hard sphere gas. On the other hand, the solution of the Boltzmann hierarchy can be formally expanded as:

$$f_k(t) = \sum_{i=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{i-1}} dt_i S_0^k(t-t_1) \mathcal{C}_{k,k+1} S_0^{k+1}(t_1-t_2) \cdots$$

$$\mathcal{C}_{k+i-1,k+i} S_0^{k+i}(t_i) f_{k+i}(0)$$

Cercignani et al. and Saint-Raymond claim that the convergence of the formal solution of the BBGKY hierarchy to the formal solution of the Boltzmann hierarchy can *only* be proved if the ingoing configurations are used:

We have *no choice* of the representation of the collision point in terms of ingoing or outgoing velocities; a representation just arises automatically, and the correct expression of the limit collision terms follows from the calculations. (Cercignani et al. 1994, p. 81. My emphasis).

And more precisely,

At this point the choice [...] to express everything in terms of pre-collisional configurations, is not really a choice. If I decide to go back from t to 0, I have *no choice*, I have to express everything in terms of pre-collisional configurations. And [...] if you would like to go from 0 to minus t [...] you have to express everything in terms of post-collisional configurations. And then, instead of the BE, what you end up with is the backward BE. [...] This is really important because this is at this point that irreversibility just enters into the game. (Saint-Raymond 2015, 43'22. My emphasis)

It is possible to use either ingoing or outgoing configurations to *express* the BBGKY hierarchy. However, it does *not* follow that “one can *derive* the Boltzmann hierarchy, as well as the anti-Boltzmann hierarchy, from the BBGKY hierarchy rewritten in terms of either the incoming or the outgoing configurations *without having to choose the “right” one.*” (Uffink and Valente 2015, p. 429. My emphases). The point I stress is that the incoming configurations are mandatory to derive the Boltzmann hierarchy, and they cannot be used to derive the anti-Boltzmann hierarchy.

5.2 Collision trees as a mathematical constraint

Cercignani et al. (1994), Gallagher et al. (2014), and Saint-Raymond (2015) emphasize that the convergence proof of the the formal solution of the BBGKY

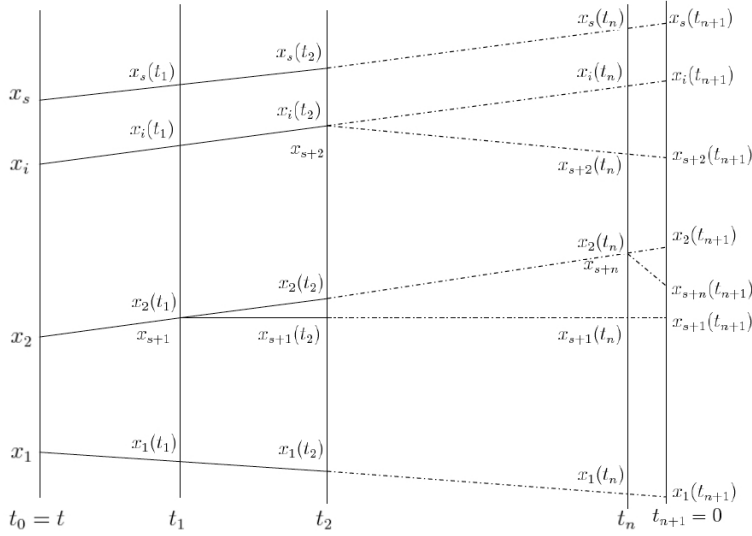


Fig. 5 Collision trees for positive times. Figure extracted from (Gallagher et al. 2014).

hierarchy $\rho_k(t)$ towards the formal solution of the Boltzmann hierarchy $f_k(t)$ is established within the framework of *collision trees*. They are graphical representations of the formal solution of the BBGKY hierarchy (see Fig. 5). For positive times, collision trees correspond to the all possible trajectories that lead to the position of a particule at the time t from an initial time. According to Saint-Raymond, within this framework, the ingoing configurations are required to prove that the formal solution of the BBGKY hierarchy converges to the Boltzmann hierarchy for positive times.¹⁰ In the same way, for negative times, the outgoing configurations are required to prove that the formal solution of the BBGKY hierarchy converges to the anti-Boltzmann hierarchy.

Cercignani et al., Gallagher et al., and Saint-Raymond claim thus that one does not know how to derive the Boltzmann hierarchy without the use of the incoming configurations. At least, as far I know, there is no rigorous derivation of the Boltzmann hierarchy without the use of the ingoing configurations. We are dealing here with a mathematical constraint that plays a crucial role in the derivation of the Boltzmann hierarchy. The use of collision trees framework comes from the use of the Duhamel formula with which the formal solution of the BBGKY hierarchy is expanded (Gallagher et al. 2014, p. 50).¹¹ The value of such a constraint is questionable. First, it seems to imply that, roughly speaking, the way that a solution is expressed would have consequences on

¹⁰ Saint-Raymond claims even more that the use of the incoming configurations is required to rigorously define the formal solution of the BBGKY hierarchy with integrals (private communication).

¹¹ This corresponds to the use of Dyson's time-dependent perturbation theory in Uffink and Valente (2015, p. 418).

the appearance of a time-asymmetric solution. This case raises more generally a philosophical issue that I will leave open here, viz. which mathematics represent physical assumptions and which ones are superfluous. Second, since the collision trees are a mathematical framework, it could possibly be removed to derive the BE. Therefore, this framework would be contingent with regard to the question of the appearance of irreversibility in the derivation of the BE. Accordingly, I do not claim that it would be impossible to derive the Boltzmann hierarchy by using outgoing configurations with *other* mathematical techniques, i.e., without the framework of collision trees. However, I stress that *as far as we are concerned* with the current Lanford's and successors's works on the BE, outgoing configurations and ingoing configurations are not equivalent with respect to the derivation of the BE.

Finally, it has to be stressed that Uffink and Valente's proof of the equivalence between the BBGKY hierarchy with incoming and outgoing configurations contrasts with such a mathematical constraint. This equivalence holds even if the BE would be derived with another framework. This makes this equivalence claim very strong. However, it holds only at the level of the BBGKY hierarchy. It is not sufficient to argue for the equivalence between ingoing and outgoing configurations at the level of the Boltzmann hierarchy.

5.3 Equivalence breaking between ingoing and outgoing configurations

I have argued that ingoing and outgoing configurations are equivalent to express the BBGKY hierarchy whereas they are *not* to derive the Boltzmann hierarchy. I stress here the role of the B-G limit regarding this difference. More precisely, I emphasize that this is the use of the B-G limit that breaks this equivalence. Therefore, the argument according to which ingoing or outgoing configurations are neutral regarding the derivation of the BE does not hold when the B-G limit is taken.

First of all, let us make clear how the equivalence between ingoing and outgoing configurations *without* the B-G limit comes from. Uffink and Valente point out that a *continuity condition about collisions* is responsible for this equivalence. This condition states that the probability density of hard spheres before collision equals the probability density of hard-spheres after collision (Uffink and Valente 2015, p. 428)¹², i.e.,

$$\rho_{k+1}(q_i, p_i; q_i + a\omega_{i,k+1}, p_{k+1}) = \rho_{k+1}(q_i, p_i'; q_i + a\omega_{i,k+1}, p_{k+1}') \quad (17)$$

This equation roughly states that the number of particles *before* colliding equals the number of particles *after* colliding. However, this equation is valid while the B-G limit is not taken yet. The equivalence of using incoming or outgoing configurations holds thus while the B-G limit is not taken yet, i.e., at the level of the BBGKY hierarchy but not at the level of the Boltzmann hierarchy. Uffink and Valente also make this point clear :

¹² See also Spohn (2006) on this point.

Let us emphasize that continuity across collisions is a peculiar condition on the BBGKY hierarchy for hard spheres, *which does not carry over when we take the Boltzmann-Grad limit*, at least if one wishes to derive a genuinely irreversible behaviour. In fact, *such a condition would have no analogue for the Boltzmann hierarchy, or the anti-Boltzmann hierarchy.* [...] [F]or an irreversible approach to equilibrium to obtain, the continuity at collisions condition, which maintains time-reversal invariance of the BBGKY hierarchy written in any collision configuration, *has no analogue in the Boltzmann-Grad limit.* (Uffink and Valente 2015, p. 429. My emphases.)

When the B-G limit is taken, we are no longer allowed to claim the equivalence between ingoing and outgoing configurations. Yet, the B-G limit is uncontroversially needed to derive the BE, and because of the use of collision trees, the ingoing configurations are also needed to derive the BE. Therefore, as a mathematical fact of Lanford's derivation, only the use of ingoing configurations within the B-G limit allows to obtain the BE. Such ingoing configurations cannot be used to derive any equations for negative times, leading to a time-asymmetry for the H -function (see Fig. 4).

6 *Stoßzahlansatz* reconsidered

This analysis of Lanford's derivation of the BE allows me to argue for a reconsideration of the *Stoßzahlansatz*, i.e., the assumption about the number of collisions in the original Boltzmann's heuristic derivation of the BE. It is generally admitted that irreversibility in Boltzmann's original derivation comes from this assumption:

[T]he irreversible time-evolution of macroscopic systems cannot be a consequence of the laws of Hamiltonian mechanics alone. There must be some additional non-dynamical ingredient in the H -theorem, or indeed in the Boltzmann equation from which it follows, that picks out a preferred direction in time. As we now know, the *Stoßzahlansatz* is the culprit. The pre-collision condition introduces a time-asymmetric element, since it is assumed to hold only for particle pairs immediately *before* collisions, but not for pairs immediately *after* they collided. (Uffink and Valente 2015, p. 410)

The time-asymmetric ingredient within the *Stoßzahlansatz* is the *pre-collision condition*, which roughly states that, at any time, particles are uncorrelated *before* collisions (Uffink and Valente 2015, p. 407).

Nevertheless, Uffink and Valente claim that the *Stoßzahlansatz* has been removed in the rigorous Lanford's derivation of the BE. More precisely, there is no longer any *pre-collision condition*. There is only a *factorization condition* but which does not make any reference to a direction of time. Indeed, the factorization condition in Lanford's derivation, corresponding to Eq. (14), is used

to obtain the BE as well the anti-BE. In other words, the factorization condition does not depend on incoming configurations or outgoing configurations, and thus does not depend on any direction in time.

However, I claim that there is actually a kind of a pre-collision condition within Lanford's derivation of the BE, because of the mandatory use of the ingoing configurations. Such ingoing configurations indeed correspond to the use of momenta of hard spheres *before* collisions. Nevertheless, if there is any new kind of *Stoßzahlansatz* within Lanford's derivation, it is different from the *Stoßzahlansatz* in Boltzmann's derivation. Unlike the original *Stoßzahlansatz*, the factorization condition in Lanford's derivation can be assumed at an initial time, and not necessarily at any time. Indeed, the factorization property at the initial time (Eq. 15) is maintained in time within Lanford's derivation, corresponding to Equation (14) at the time t . This property is called the *propagation of chaos* (Uffink and Valente 2015, p. 418).

In other words, according to my analysis of Lanford's derivation of the BE, one can roughly view the hard spheres of the gas as assumed, *before* collisions (because of the mandatory use of the incoming configurations), to be *uncorrelated at the initial time* (because of the factorization condition).

7 Conclusion

Based on Uffink and Valente's paper (2015), I discussed the problem of the appearance of irreversibility in Lanford's and successors' derivation of the Boltzmann equation (Lanford 1975, Cercignani et al. 1994, Gallagher et al. 2014). Unlike Uffink and Valente, I claimed that there is a time-asymmetric ingredient that, added to the Hamiltonian equations of motion, allows to obtain the Boltzmann equation. Such a time-asymmetric ingredient is the use of incoming configurations as taken within the Boltzmann-Grad limit.

Following Uffink and Valente's analysis, I first clarified that the Boltzmann-Grad limit and the incoming configurations are not, by themselves, time-asymmetric ingredients. In addition, each of them is essential for Lanford's derivation of the Boltzmann equation. Nevertheless, I emphasize that incoming configurations and outgoing configurations are *not* neutral with respect to the derivation of the Boltzmann equation. Outgoing configurations can be used to *express* the BBGKY hierarchy – before using the Boltzmann-Grad limit – but not to *derive* the Boltzmann hierarchy, and therefore the Boltzmann equation. I thus stressed that one cannot dispense with incoming configurations to derive the Boltzmann equation, at least as far as we are concerned with the current Lanford's derivation. Accordingly, I suggest that there is a kind of pre-collision condition in this derivation. However, there is no Boltzmann's *Stoßzahlansatz* within this derivation since the factorization condition can be assumed for a single initial time.

Acknowledgements

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