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Irreversibility in the derivation of the Boltzmann equation

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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 reply to that analysis. I claim that there are two main ingredients in the derivation of the Boltzmann equation with regard to the question of irreversibility. On the one hand, the use of the Boltzmann-Grad limit allows to derive equations that are *not* invariant under time reversal from equations that are time reversal invariant. On the other hand, the choice of incoming configurations instead of outgoing configurations to represent collisions between particles, is the time-asymmetric ingredient allowing to obtain the Boltzmann equation.

Keywords Boltzmann equation · Lanford's theorem · Boltzmann-Grad limit · irreversibility · time-reversal invariance

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 this 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 Boltzmann-Grad limit, nor the incoming configurations are responsible for the appearance of irreversibility in the derivation of the BE. I argue that their analysis is, at some points, misleading and I discuss how irreversibility appears within Lanford's derivation.

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). Second, I investigate the role of the B-G limit in the derivation of BE (Section 3). Uffink and Valente mitigated its role in the appearance of irreversibility. I show why their analysis is misleading and emphasize that the B-G limit allows to derive equations that are not invariant under time reversal from time reversal invariant equations. Then, I turn to the role of incoming configurations in the derivation of the BE (Section 4). I argue that they are the time-asymmetric ingredient allowing to obtain the BE from the Hamiltonian equations of motion.

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 density of the probability 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

[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 0. See Section 2.2 of the paper.

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 recently completed by 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 to introduce 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:

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

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

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:

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

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

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

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]

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[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.

[4] Indeed, two particules 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.

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

$$H(f_t) = \int f_t(q,p) \ln f_t(q,p) dp dq \tag{5}$$

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 $\mu(x_1, x_2, ..., x_N)$ in the phase space:

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

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:

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

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

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

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

with

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

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

Step 2: From the BBGKY hierarchy to the Boltzmann hierarchy

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

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

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

$$\mathcal{C}_{k,k+1} f_{k+1,t} = \tag{11}$$

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

$$\big[f_{k+1,t}(x_1, ..., q_i, p_i{}', ..., q_i, p'_{k+1}) - f_{k+1,t}(x_1, ..., q_i, p_i, ..., q_i, p_{k+1})\big] \tag{13}$$

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 :

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

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:

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

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

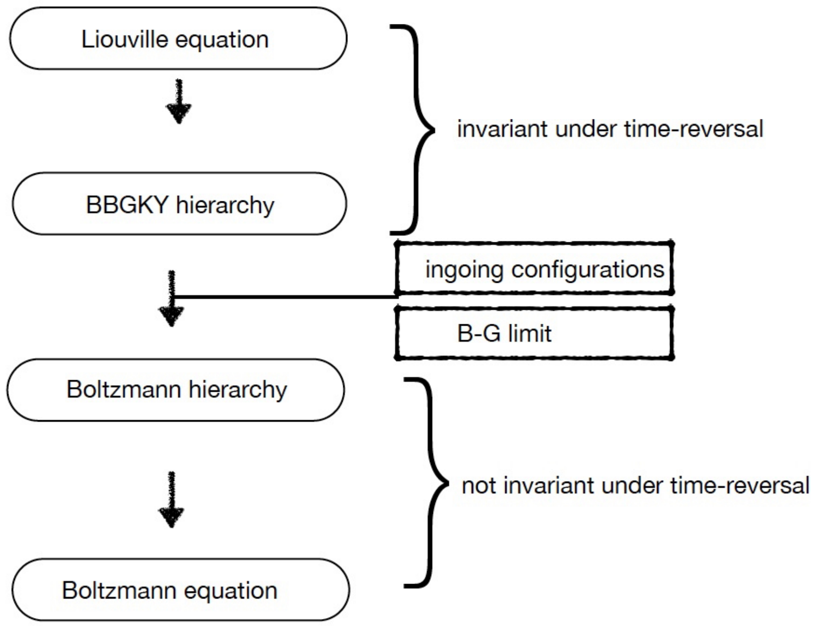

Fig. 1 Main steps of Lanford's derivation of the Boltzmann equation.

2.3 The question of irreversibility within Lanford's theorem

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 when 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). In Section 3, I will argue accordingly that the B-G limit contributes to account for the appearance of irreversibility within Lanford's derivation – even if it is not a time-asymmetric ingredient.

Second, 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 $\mathcal{C}^{(a)}_{k,k+1}$ of the BBGKY hierarchy in order to obtain the collision term $\mathcal{C}_{k,k+1}$ of the Boltzmann hierarchy. Such configurations contrast with outgoing configurations, which are the momenta *after* collision, also called post-collisional configurations. But, because of 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. However, as we will see in Section 4, ingoing but not outgoing configurations are required to derive the BE. Accordingly, I will argue that they are the time-asymmetric ingredient for the appearance of irreversibility.

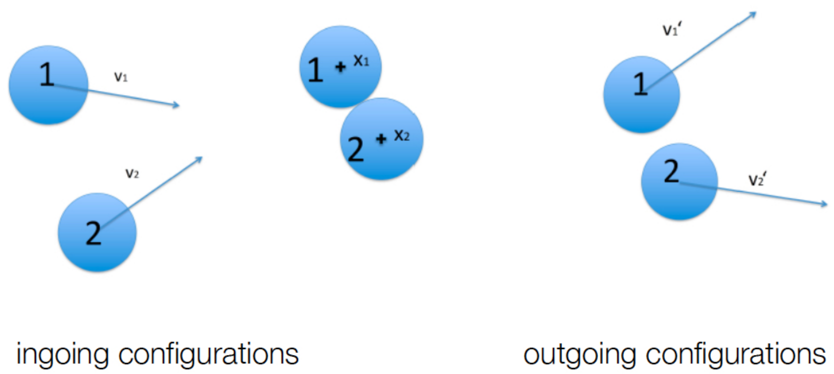

Fig. 2 Ingoing and outgoing configurations. Figure extracted from (Saint-Raymond 2013).

Uffink and Valente (2015) claimed 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 addressed 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):

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

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.

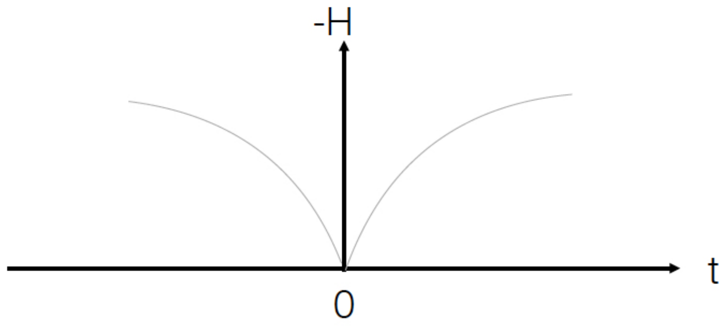

Fig. 3 Time-symmetry of H-theorem derived from Lanford's theorem.

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 4, the use of 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 4 that ingoing configurations are the time-asymmetric ingredient that allows to derive the BE from Hamiltonian equation of motions. But before that, I investigate in Section 3 the role of the B-G limit in the appearance of irreversibility.

3 The Boltzmann-Grad limit

In his seminal paper, Lanford (1975, p. 110) points out that irreversibility appears in derivation of the BE when the B-G limit is taken. More precisely, he emphasizes that the B-G limit allows to derive the Boltzmann hierarchy, which is not time-reversal invariant from the BBGKY hierarchy, which is invariant under time-reversal. However, Uffink and Valente (2015, p. 424) mitigate the role of the B-G limit for the appearance of irreversibility based on a comparison made by Lanford (1981, p. 75) himself between the derivation of the BE and the derivation of the Vlasov equation (VE). This section aims at showing that Uffink and Valente's argument is misleading. Contrary to what they suggest, I argue that the derivation of the VE does not require the B-G limit. One thus cannot draw any conclusions about the B-G limit based on an analysis of the derivation of the VE. Then, I make clear that the B-G limit plays an important role in the appearance of irreversibilty since it breaks the time-reversal invariance of the BBGKY hierarchy, even though it is not a time-asymmetric ingredient in the derivation of the BE.

3.1 The mitigated role of the Boltzmann-Grad limit

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. He illustrated this by the Vlasov equation"(2015, p. 424. My emphasis). In this section, I make clear why, at first glance, Uffink and Valente would apparently be right to mitigate the role of the B-G limit for the appearance of irreversibility.

Let us introduce the VE and compare it with the BE. 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 :

$$\phi^{(N)}(q_1 - q_2) = \frac{1}{N}\phi_0(q_1 - q_2) \tag{17}$$

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 :

$$\frac{\partial}{\partial t} f_t(q,p) + \frac{p}{m} \cdot \frac{\partial}{\partial q} f_t(q,p) = -\mathcal{F}(q)\frac{\partial}{\partial p} f_t(q,p) \tag{18}$$

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.

Nevertheless, as Lanford (1981) points out, both 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. This contrasts with the case of the BE for which its H-function monotonically decreases with time. Therefore, there are two macroscopic equations derived from N-body systems with $N \to \infty$ that exhibit irreversibility or do not exhibit irreversibility. That is the reason of why Uffink and Valente mitigate the role of the B-G limit for the appearance of irreversibility.

3.2 Boltzmann-Grad limit and effective field limit

Contrary to what Uffink and Valente (2015) suggest, the derivations of the BE and the VE are actually based on two different limiting regimes. The BE is derived with the *B-G limit* although the VE is derived with a limit called the *effective field limit*, also called *mean field limit.*

First of all, unlike the BE, the VE is 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). Indeed, the derivations of the BE and the VE are based on two different idealizations about how particles interact with each other: the derivation of the BE assumes a *strong but local* coupling between particles, which corresponds to a collisional model. Such assumption occurs generally within a hard spheres model (but it is not restricted to this case). Instead, 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 macroscopic in the sense that two particles which are far from each other still interact with each other. When $N \to \infty$, one obtains a mean field approximation, which leads to the VE.[5]

More to the point, the derivation of the VE does not require the B-G limit. It requires the effective field limit which only needs that $N \to \infty$ in order to scale the strength of interactions. Instead, the derivation of the BE requires the B-G limit, which needs in addition that $a \to 0$ in order to scale the range of interactions, where Na^2 is a finite quantity. In the derivation of the VE, the diameter a of hard spheres is not a limit parameter. The VE is indeed derived from a model of N mass points, which implies that particles have already zero diameter when N is finite. One could object that the BE can be also derived from a model of N mass points. In this case, two mass points interact with a short-range repulsive potential (King 1975, Gallagher et al. 2014). But this derivation of the BE still requires the B-G limit: It requires the $N \to \infty$ limit and the $a \to 0$ limit for which a is now the range of a short-range repulsive potential.[6]

[5] In addition, the derivations of the VE and the BE require two different notions of convergence.

[6] Norton (2012, p. 218) points out that extensionless points with the B-G limit are problematic with respect to determinism. When $a \to 0$ 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 $a \to 0$. Besides, 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 $r \to 0$ [i.e. $a \to 0$]. 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 $r \to 0$, the definition of the collision integral [...] requires the

These two limiting regimes, i.e., the B-G limit and the effective field limit, are two ways 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 can be done "either by scaling the strength of the force, or by scaling the range of potential"(Gallagher et al. 2014, p. 7). The first case leads to the VE and the second one to the BE. But, even if both equations are derived from Hamiltonian equations of motion in the limit when N tends to infinity, only the second one is a collisional model.

The way that Lanford (1981, p. 76) concludes his paper is very informative about the alleged mitigated role of the B-G limit for the appearance of irreversibility:

> Why are the two limiting regimes so different with regard to irreversibility? I don't know a really good answer to this question [...]. The only lesson I want to draw from all this is that the mere fact that a macroscopic description is related to the microscopic one through a coarse-graining formalism [...] does not in itself suffice to guarantee that the macroscopic theory will display irreversibility.

First of all, Lanford himself makes clear that the BE and the VE are derived from two different limiting regimes. Second, I stress that Lanford draws only a single lesson from his comparison between the derivation of the BE and the VE. This lesson does not pertain to the role of the B-G limit in particular. It pertains more generally to all procedures that give a macroscopic description of a N-body system. Lanford only concludes that using a limiting regime in order to derive a macroscopic equation from Hamiltonian equations of motion does not guarantee that the macroscopic equation will be non invariant under time-reversal. This is precisely what the derivation of the VE shows. But one should not conclude that the role of the B-G for the appearance of irreversibility has to be mitigated.

3.3 The break of time-reversal invariance

Until now, my claim was essentially negative: we cannot argue that the B-G limit is not sufficient for the appearance of irreversibility from the analysis of the VE.[8] In this section, I emphasize the role of the B-G with regard to the question of irreversibility.

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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.

[8] The derivation of the VE is still informative about the role of the $N \to \infty$ limit. Since this derivation requires the $N \to \infty$ limit, I agree with Uffink and Valente (2015, p. 424) who notice the $N \to \infty$ limit is compatible with the derivation of a macroscopic equation which is time-reversal invariant.

Uffink and Valente make perfectly clear that the B-G limit is required in the second step of the derivation of the BE (Section 2.3). It is used to derive the Boltzmann hierarchy from the BBGKY hierarchy. Accordingly, I stress that the B-G limit allows to break the time reversal invariance of the BBGKY hierarchy: it allows to derive equations that are non invariant under time-reversal from time-reversal invariant equations. However, I do not claim that the B-G limit is a time-asymmetric ingredient. Indeed, as we have seen in Section 2.3, the B-G limit is also used to derive the anti-BE. For negative times, the B-G limit is used to derive an anti-Boltzmann hierarchy, which is also not invariant under time-reversal form the BBGKY hierarchy. The B-G limit is thus used within Lanford's theorem, which is time-symmetric. But my point is that the B-G limit is undeniably involved in breaking time reversal invariance of the BBGKY hierarchy, for both positive and negative times. In that sense, the B-G limit *contributes* for the appearance of irreversibility. It is not a sufficient ingredient, since Lanford's theorem is time-symmetric, but it is still an ingredient that allows to break time-reversal invariance of the BBGKY hierarchy. Now, I shall argue that there is another ingredient in the derivation of the BE that completes the appearance of irreversibility, which is the use of the incoming configurations to represent collisions (Section 4).

4 Incoming 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. There is a debate about the role of incoming configurations with regard to the appearance of irreversibility. On the one hand, Lanford (1975) and Cercignani et al. (1994) argue that this representation is mandatory to derive the BE. On the other hand, Uffink and Valente argue against this claim. They argue that the use of incoming configurations or outgoing configurations is neutral with respect to the derivation of the BE. In this section, I make clear the role of incoming configurations in the derivation of the BE. In agreement with Lanford, and Cerxignani et al. I claim that the incoming configuration are mandatory to derive the BE and, accordingly, they are a time-asymmetric ingredient that allows to obtain the Boltzmann equation.

This section is organized as follows. First, I introduce the debate on the incoming configurations (Section 4.1). Then, I argue for the mandatory use of the incoming configurations in the derivation of the BE (Section 4.2).

4.1 The debate about ingoing and outgoing configurations

A crucial step in the derivation of the BE 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 $\mathcal{C}^{(a)}_{k,k+1}$ (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 seems to lie on the use of the incoming representation.

Nevertheless, Uffink and Valente reject this account:

> 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 with incoming momenta and the BBGKY hierarchy with the collision term expressed with outcoming momenta (2015, p. 435). This result seems in contradiction with the position of Cercignani et al. who emphasize that, at some point of the derivation, "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). At this point of the debate, either Lanford and Cercignani on the one hand or Uffink and Valente on the other hand are wrong, either what they state is still compatible. I argue for the second option.

4.2 The mandatory use of the ingoing configurations

I claim 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 the first sentence of the previous quote of Uffink and Valente. Nevertheless, ingoing and outgoing configurations are not equivalent to *derive* the Boltzmann hierarchy, and respectively to derive the backward Boltzmann hierarchy.

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:

$$\rho_k(t) = \sum_{i=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{i-1}} dt_i S_a^k(t-t_1) \; \mathcal{C}^{(a)}_{k,k+1} S_a^{k+1}(t_1-t_2) \cdots \mathcal{C}^{(a)}_{k+i-1,k+i} S_a^{k+i}(t_i) \rho_{k+i}(0)$$

where $S_a(.)$ 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:

> 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. I perfectly agree with Uffink and Valente on this point, which is clearly stated in the *Proposition 3* of their paper (Uffink and Valente 2015, p. 435). As they emphasize, this equivalence comes from a continuity condition about collisions, which 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)[9]:

$$\rho_{k+1}(q_i, p_i; q_i + a\omega_{i,k+1}, p_{k+1}) = \rho_{k+1}(q_i, {p_i}'; q_i + a\omega_{i,k+1}, p_{k+1}') \tag{19}$$

This equations roughly states that the number of particles *before* colliding equals the number of particles *after* colliding. But this equation is only 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 when they 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" (p. 429).

However, Saint-Raymond (2015) and Cercignani et al. (1994) emphasize that, in order that the solution of the BBGKY hierarchy $\rho_k(t)$ formally converges to the solution of the Boltzmann hierarchy $f_k(t)$, the use of the ingoing configuration is required.[10] This convergence is proved within the framework

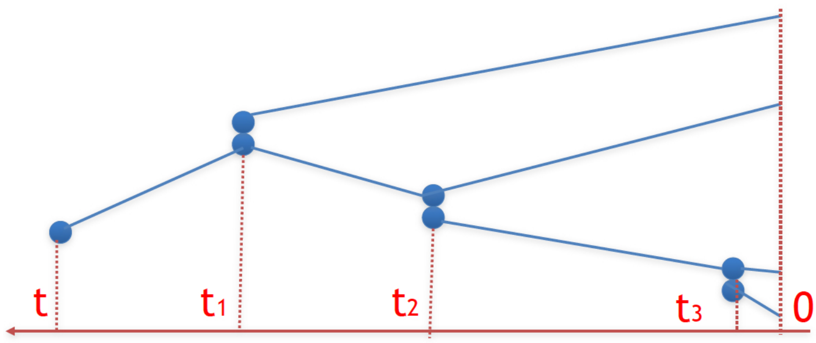

Fig. 4 Collision trees for positive times. Figure extracted from (Saint-Raymond 2013).

of collisions trees, which are graphical representations of the formal solution of the BBGKY hierarchy. For positive times, collision trees correspond to the

[9] See also (Spohn 2006) on this point.

[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).

all possible trajectories that lead to the position of a particule at the time t. 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. In the same way, for negative times, the outgoing configurations are required to prove that the formal solution of the BBKY hierarchy converges to the anti-Boltzmann hierarchy. Uffink and Valente are right when they claim that the BBGKY hierarchy can be equally rewritten with the incoming or the outgoing configurations. 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"(Uffink and Valente 2015, p. 429). And indeed, Cercignani et al. and Saint-Raymond claim 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 proof that the Boltzmann hierarchy can be derived without the use of the ingoing configurations. This is a main point of my argument. I do not claim that it would not be possible, with *other* mathematical techniques (i.e., without the framework of collision trees), to derive the Boltzmann hierarchy by using outgoing configurations. But as far as we are concerned with the actual Lanford's and successors's derivation of the BE, outgoing configurations and ingoing configurations are merely *not* equivalent.

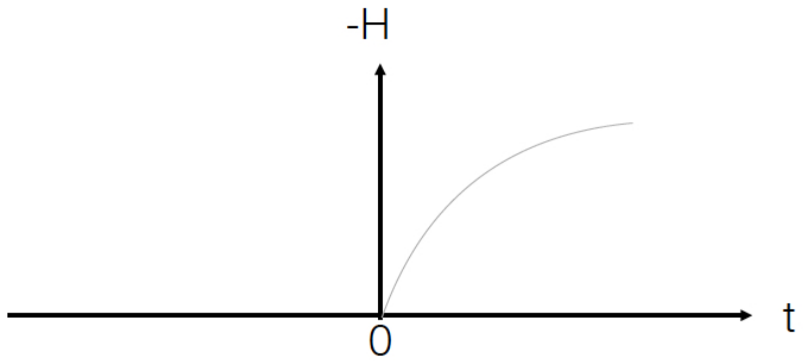

Fig. 5 H-theorem with incoming configurations and without outgoing configurations.

The use of incoming configurations add thus a time-asymmetric ingredient in the derivation of the BE because collisions are represented by momenta *before* collision. Moreover, it breaks the time-symmetry of Lanford's derivations of both BE and anti-BE. Indeed, if we *only* use ingoing configurations, one can (i) derive the BE for positive times within Lanford's theorem but (ii), for negative times, nothing can be derived. Accordingly, one has only an increasing minus H function for positive times and nothing for negative times. Unlike the H function in Fig 3, the H function is no longer time-symmetric (Fig. 5). In that sense, the incoming configurations are the time-asymmetric ingredient in the derivation of the BE.

5 Conclusion

Based on Uffink and Valente's paper (2015), I discussed the problem of the appearance of irreversibility in Lanford's and successors' (Cercignani et al. 1994, Gallagher 2014) derivation of the Boltzmann equation. Contrary to what Uffink and Valente claim, I argued that there is a time-asymmetric ingredient that, added to the Hamiltonian equations of motion, allows to obtain the Boltzmann equation.

More precisely, I have first stressed that one should not mitigate the role of the Boltzmann-Grad limit with regard to the appearance of irreversibility from an analysis of the Vlasov equation. The derivation of this latter equation indeed does not require the Boltzmann-Grad limit. However, I agree with Uffink and Valente when they emphasize that the Boltzmann-Grad limit allows to derive equations that are *not* invariant under time reversal from equations that are invariant under time reversal. This is a first step – but not a sufficient step – towards the appearance of irreversibility. Second, I argued that incoming configurations – or pre-collisional configurations – are the time-asymmetric ingredient allowing to obtain the Boltzmann equation. Unlike Uffink and Valente, I argued that incoming configurations and outgoing configurations are *not* neutral with respect to the derivation of the Boltzmann equation. My point is that 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. Incoming configurations and outgoing configurations would be equivalent if one could derive the Boltzmann equation by using either incoming configurations or outgoing configurations. However, as far as we are concerned with the mathematical techniques actually used in Lanford's and successor's derivation, this is not the case. One cannot dispense with incoming configurations to derive the Boltzmann equation.

Acknowledgements

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