On the Boltzmann-Grad limit of the Master Kinetic Equation

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In this paper the problem is posed of the prescription of the so-called Boltzmann-Grad (BG) limit ($\mathcal{L}_{BG}$) for the $N$--body system of smooth hard-spheres which undergo unary, binary as well as multiple elastic instantaneous collisions. The statistical description is couched in terms of the Master kinetic equation, i.e., the kinetic equation which realizes the axiomatic “ab initio” approach to the classical statistical mechanics of finite hard-sphere systems recently developed (Tessarotto et al., 2013-2017). The issue addressed here concerns the prescription of the BG-limit operator and specifically the non-commutative property of $\mathcal{L}_{BG}$ with the free-streaming operator which enters the same kinetic equation. It is shown that the form of the resulting limit equation remains in principle non-unique, its precise realization depending critically on the way the action of the same operator is prescribed. Implications for the global prescription of the Boltzmann equation are pointed out.

1- INTRODUCTION

The Boltzmann kinetic equation \cite{1,2} is commonly regarded as a cornerstone of classical statistical mechanics (CSM). Its applications are widespread ranging from the kinetic description of rarefied gases and plasmas to particle simulation methods for continuous fluid systems, such as the Lattice-Boltzmann \cite{3,4} and smoothed-particle hydrodynamics methods \cite{5}. It also serves as a tool for the rigorous derivation of hydrodynamic equations which (hopefully) should hold globally in time (i.e., for all $t$ belonging to the time axis $I \equiv \mathbb{R}$) for a variety of fluid systems \cite{6}, including in particular Navier-Stokes fluids \cite{7}. Both the 1--body phase-space construction of the equation given by Boltzmann and the corresponding $N$--body phase-space statistical treatment based on CSM later given by Grad actually refer to the closed $N$--body system $S_N$ formed by identical hard spheres of diameter $\sigma$ subject to instantaneous elastic collisions. By assumption they are immersed in a stationary bounded and connected configuration domain $\Omega$ subset of the Euclidean space $\mathbb{R}^3$, for example identified with a cube of measure $\mu(\Omega) = L^3_0$. Hereon, for definiteness, the 1--body phase-space spanned by the single-particle Newtonian state $x_1 \equiv \{r_1, v_1\}$ will be identified with $\Gamma_1 = \Omega \times U_1$ (being $U_1 = \mathbb{R}^3$ the related velocity space), while $x \equiv \{x_1, \ldots, x_N\}$ and $\Gamma_N \equiv \prod_{i=1}^{N} \Gamma_{1(i)}$ are the corresponding $N$--body system state and the $N$--body phase-space. Despite its fundamental relevance the Boltzmann equation has been for a long time plagued by issues and criticism related to both statistical approaches. Some of them, rather surprisingly, have remained unsolved to date or until very recently, thus possibly hindering subsequent meaningful developments of kinetic theory itself. Some of them are historically-famous. These include the Loschmidt \cite{8} and Zermelo \cite{9} objections to Boltzmann H-theorem, both in its original formulation \cite{10} and in its modified form introduced by Boltzmann himself while attempting to reply to Loschmidt objection \cite{10} (see also Refs. \cite{11,12} together with different views on the matter given in Refs. \cite{13,14}). Other no less important and well-known issues are related to physical conditions of validity of the Boltzmann equation \cite{15}, its possible generalization to the treatment of finite-size and dense hard-sphere systems \cite{16} as well the prescription adopted both by Boltzmann and Grad regarding the so-called collision boundary conditions (CBC) for the $N$--body probability density function (PDF) \cite{17}. More precisely this concerns the prescription for arbitrary collision events of the relationship between incoming ($-$) and outgoing ($+$) PDFs, i.e., respectively the left and right limits $\rho^{(\pm)}(x^\pm(t_i), t_i) = \lim_{t \to t_i^\pm} \rho^{(N)}(x(t), t)$, with...
\(x^{(\pm)}(t_i) = \lim_{t \to t_i^\pm} x(t)\) denoting the corresponding incoming (-) and outgoing (+) states. Indeed in these approaches (see also Ref. [17]) the CBC is identified with the PDF-conserving CBC

\[
\rho^{(-)(N)}(x^{(-)}(t_i), t_i) = \rho^{(+)(N)}(x^{(+)}(t_i), t_i),
\]

where upon invoking causality the assumption of left-continuity, i.e., the requirement

\[
\rho^{(-)(N)}(x^{(-)}(t_i), t_i) \equiv \rho^{(N)}(x^{(-)}(t_i), t_i)
\]

is usually implicitly adopted for the causal realization of PDF-conserving CBC (see e.g. [17]).

In connection with the first-principle construction of the Boltzmann equation based on CSM, however, a further issue must be mentioned. This is about the prescription of the so-called Boltzmann-Grad limit (BG-limit) first explicitly introduced by Grad [2] but actually set at the basis of Boltzmann’s construct of his namesake kinetic equation [1]. In this letter we intend to point out crucial aspects involved in its prescription in the context of the "ab initio“ axiomatic approach for hard-sphere systems [12, 27, 34] and the related discovery of the Master kinetic equation for hard spheres undergoing elastic instantaneous mutual collisions [28, 30–32]. The problem is in fact physically relevant for two main reasons, i.e., to establish a rigorous connection with the Master kinetic equation itself and in order to ascertain whether and under which conditions the Boltzmann equation can be exactly recovered in an appropriate asymptotic limit.

To start with it is well known that Boltzmann himself was well aware of the finite size (and finite number) of molecules occurring in real gases [18] (see also Ref. [19]). Nevertheless there it emerges clearly that he also regarded the BG-limit as a mandatory requirement. Indeed, according to Boltzmann’s own original statement his equation should not be regarded as "... precisely correct ... (if) the number of particles (N) is not ... infinite" [20], i.e., only when the continuum limit

\[
N \equiv \frac{1}{\varepsilon} \to \infty
\]

is evaluated, while requiring simultaneously "a decreasing size of the molecules" [21]. In doing so, he implicitly assumed also that the configuration domain \(\Omega\) should remain unaffected by the BG-limit, thus implying that the ordering

\[
L_0 \sim O(\varepsilon^0)
\]

should apply too. In Grad’s treatment the same conditions are set in a mathematically more precise form in terms of normalized lengths, in particular the normalized particle diameter \(\overline{r} \equiv \frac{1}{L_R}(L_R\) being a suitable, but unspecified, reference scale length implicitly taken of order \(L_R \sim O(\varepsilon^0)\)). For this purpose he required that in the continuum limit the ordering condition

\[
N\overline{r}^2 \sim O(\varepsilon^0)
\]

should apply both to the kinetic equation and to the equations of the related BBGKY hierarchy for hard-sphere systems implicitly assuming also [10].

The proof of the existence of the BG-limit, given by Lanford [23, 24] and usually referred to as Lanford theorem [23], shows that under certain conditions the Boltzmann equation can be obtained from the same BBGKY hierarchy by suitably applying to it an appropriate limit operator denoted as BG-operator \(\mathcal{L}_{BG}\). However, according to Villani [26] “...present-day mathematics”, and in particular Lanford theorem, is actually “...unable to prove (such a result) rigorously and in satisfactory generality” the obstacle being that it is not known “...whether solutions of the Boltzmann equation are smooth enough, except in certain particular cases”.

Nevertheless additional serious questions arise which need to be carefully taken care of. These are related to the definition of the same limit operator, the conditions of validity of the BG-limit and the possible occurrence of a non-commutative product behavior with respect to differential operators occurring in the same context, i.e., the (possible) coincidental non-uniqueness in the prescription of the same BG-limit itself. A feature of this type would not be completely unexpected indeed. It occurs, for example, for the so-called thermodynamic limit obtained invoking the continuum limit [23] together with the ordering \(\varepsilon \to O(\varepsilon^0)\). In this case, in fact, it is well known that the corresponding limit operator \(L_{ther}\) may not commute with the partial derivative with respect to extensive thermodynamic variables such as the volume \(V\), so that in particular it may occur that \(\frac{\partial}{\partial \varepsilon} L_{ther} \neq L_{ther} \frac{\partial}{\partial \varepsilon} [22]\).

More precisely, besides the identification of the conditions warranting the global existence of the BG-limit, the issue to be addressed refers to the precise mathematical prescription of how it acts on the equations of the BBGKY hierarchy for hard-sphere systems and the properties of the corresponding multi-body PDFs. These features affect, in turn, also the possible non-commutative property of its ordered products with respect to the 1-body free-streaming differential operator \(L_1 \equiv \frac{1}{\overline{r}^2} + \mathbf{v}_1 \cdot \frac{\partial}{\partial \mathbf{r}_1}\), whereby it may result that

\[
\mathcal{L}_{BG} L_1 \neq L_1 \mathcal{L}_{BG}.
\]

Thus the identification of these properties of \(\mathcal{L}_{BG}\) is of critical importance because of the (possible) non-uniqueness of the BG-limit and the consequent need to prescribe also the precise order in which the product of the operators \(\mathcal{L}_{BG}\) and \(L_1\) should be taken.

It is obvious that the issues indicated above about the BG-limit have potentially serious implications. In fact they concern, ultimately, the conditions of validity of the Boltzmann equation itself as well as its actual relevance for the statistical description of rarefied gases. To resolve them in the following we shall adopt the Master kinetic equation [28] and the related microscopic statistical description of hard-sphere systems [24], both based on
the recently-developed "ab initio" axiomatic approach to CSM [15, 27, 34]. The new statistical approach actually deals, just as those due to Boltzmann and Grad, with a closed $N$–body system $S_N$ of smooth hard-spheres which are subject to elastic instantaneous unary, binary and multiple collisions. Nevertheless the novelty of the "ab initio" approach lies in the fact that it permits the treatment of finite hard-sphere $N$–body systems, i.e., in which both the number of particles $N$ and their diameter $\sigma$ remain finite. To achieve such a goal suitably-prescribed physical prerequisites are introduced. More precisely, departing from Boltzmann and Grad original statistical approaches, these concern, first, the functional setting for the $N$–body PDF $\rho^{(N)}(x, t)$, the obvious physical requirement being that the same must include ordinary functions as well as distributions, such as in particular the so-called certainty function [35], i.e. the deterministic $N$–body Dirac delta $\rho^{(N)}_{B}(x, t) \equiv \delta(x - x(t))$ [15]. Second, to warrant validity of the same functional setting, a suitable physically-prescribed realization must be adopted also for the CBC of the $N$–body PDF. In particular, upon invoking again due to causality the assumption of left-continuity [2], the incoming PDF is required to coincide with the same $N$–body PDF evaluated in terms of the incoming state and time since the same relationship must obviously apply also to $N$–body deterministic PDF $\rho^{(N)}_H(x, t)$, one can show [15, 27] that the so-called causal form of the modified collision boundary conditions (MCBC [27])

$$\rho^{(+)(N)}(x^{(+)}(t_i), t_i) = \rho^{(N)}(x^{(+)}(t_i), t_i)$$

is mandatory. This warrants that along an arbitrary Lagrangian trajectory the functional form of the PDF, such as the $N$–body Dirac delta, remains unaffected by arbitrary unary, binary and multiple collisions. The validity of MCBC, as shown in Ref. [28], is of key importance since it permits the global existence [32] of an exact particular solution of the $N$–body Liouville equation identified with the factorized $N$–body PDF

$$\rho^{(N)}(x, t) = \overline{\sigma}^{(N)}(x) \prod_{i=1}^{N} \tilde{\rho}^{(N)}_{1}(x_i, t),$$

so that for all $s = 1, N - 1$, the corresponding $s$–body PDF $\rho^{(N)}_{s}(x) \equiv \rho^{(N)}(x_i, x_i, x_i, \ldots)$ is

$$\rho^{(N)}_{s} = \overline{\sigma}^{(s)}(x) \prod_{i=1}^{s} \tilde{\rho}^{(N)}_{1}(x_i, t) k^{(N)}_{s}(r_1, \ldots, r_s, t).$$

Here the notation is standard [28, 32], with $\overline{\sigma}^{(N)}(x) \equiv \prod_{i=1}^{N} \tilde{\sigma}^{(x)}_{i}(x_i)$ being the ensemble theta function, i.e., prescribing the admissible subset of the $N$–body phase space $\Gamma^{(N)}$, and similarly $\overline{\sigma}^{(s)}(x) = \prod_{i=1}^{s} \tilde{\sigma}^{(x)}(x_i)$. Thus, in particular

$$\overline{\sigma}^{(1)}_{i}(x_i) \equiv \overline{\sigma}^{(1)}_{i}(x_i) \overline{\sigma}^{(1)}(x_i)$$

with $\overline{\sigma}^{(1)}_{i}(x_i) \equiv \overline{\sigma}(|x_i - x_{W_i}| - \frac{\sigma}{2})$ and $\overline{\sigma}(x)$ being everywhere the strong theta function. Furthermore in $\overline{\sigma}^{(0)}(x), r_{W_i} = r_i - \frac{\sigma}{2} n_i$ and $\overline{\sigma}(x)\tilde{\sigma}(x)$ denote the inward vector normal to the boundary belonging to the center of the $i$–th particle having a distance $\frac{\sigma}{2}$ from the same boundary. Next, in the product $\prod_{i=1}^{N} \tilde{\rho}^{(N)}_{1}(x_i, t)$, $\rho^{(N)}_{1}(x_i, t)$ and $\tilde{\rho}^{(N)}_{1}(x_i, t)$ identify respectively the 1–body PDF and its renormalized form

$$\tilde{\rho}^{(N)}_{1}(x_i, t) \equiv \frac{\rho^{(N)}_{1}(x_i, t)}{k^{(N)}_{1}(r_1, t)},$$

while $k^{(N)}_{1}(r_1, t)$ denotes the 1–body occupation coefficient prescribed so that $\rho^{(N)}(x, t)$ is normalized to unity. By construction this means that denoting $\Gamma^{N-1} = \prod_{i=2}^{N} \Gamma_{1(i)}$, in Eq. (8) the corresponding $s$–body occupation coefficient is

$$k^{(N)}_{s}(r_1, \ldots, r_s, t) = \int_{\Gamma^{N-s+1}_{s+1}} dx_i \tilde{\rho}^{(N)}_{1}(x_i, t) \overline{\sigma}^{(s)}_{s}(r_1, \ldots, r_s, t).$$

The remarkable implication of the factorized solution $\rho^{(N)}(x, t)$ is the global validity of an exact kinetic equation which advances in time the same 1–body PDF. This is provided by the Master kinetic equation which can be represented in two equivalent forms (see Ref. [28]), the first one being

$$L_{1} \tilde{\rho}^{(N)}_{1}(x_1, t) = 0,$$

where $L_{1} = \frac{\partial}{\partial t} + v_i \cdot \frac{\partial}{\partial x_i}$ denotes the 1–body free-streaming operator. As shown in Ref. [28] this equation can be cast in a form formally similar to the Enskog kinetic equation. Nevertheless Eq. (13) differs radically from either the Enskog or Boltzmann kinetic equations, at least for the following basic implications, i.e.

\begin{itemize}
  \item The non-asymptotic character of the Master kinetic equation [28, 30]. In fact the same equation realizes also an exact particular factorized solution of the $N$–body Liouville equation. As such it holds also in the case of $N$–body systems formed by a finite number $N \geq 2$ of finite-size ($\sigma > 0$) smooth hard spheres which undergo elastic (unary, binary or multiple) instantaneous mutual collisions.
• The exact determination of the configuration-space multiparticle correlations [28]. Indeed, the form of the factorized \( s \)-body PDF \( \rho_s^{(N)} \) for all \( s = 2, N \), prescribed according to Eq. (39), determines uniquely the corresponding form of the \( s \)-body correlation function in the \( s \)-body phase space \( \Gamma^s = \prod_{i=1,s} \Gamma_{1(i)} \). This is provided by \( \Delta \rho^{(N)}_s = \Delta \rho^{(N)}_s(\mathbf{x}_1,\ldots,\mathbf{x}_s,t) \) with

\[
\Delta \rho^{(N)}_s = \rho^{(N)}_s - \Theta^{(s)}(\mathbf{r}) \prod_{i=1,s} \rho^{(N)}_{1,i}(\mathbf{x}_i,t).
\]

• Constant H-theorem \[31\]. Thus, denoting by \( S(\rho^{(N)}_1(t)) = -\int d\mathbf{x}_1 \rho^{(N)}_1(\mathbf{x}_1,t) \ln \rho^{(N)}_1(\mathbf{x}_1,t) \) the Boltzmann-Shannon (BS) entropy functional and assuming that the initial PDF

\[
\rho^{(N)}_{1} (\mathbf{x}_1,t_o) \equiv \rho^{(N)}_{1(o)} (\mathbf{x}_1),
\]

admits the BS-functional \( S(\rho^{(N)}_1(t_o)) \) it follows necessarily \[31\] that for all \( t \in I \), \( \rho^{(N)}_{1} (\mathbf{x}_1,t) \) admits the same functional \( S(\rho^{(N)}_1(t)) \) and fulfills identically the constant H-theorem

\[
S(\rho^{(N)}_1(t)) = S(\rho^{(N)}_1(t_o)).
\]

• Global validity of solutions of the Master kinetic equation. In Ref. [32] the global existence for the Master kinetic equation was established based on the validity of MCBC and on the existence of global factorized solutions of the form (7) for the corresponding \( N \)-body Liouville equation. An example of global particular solutions of the Master kinetic equation (see Ref. [32]) is provided by \( 1 \)-body PDFs \( \rho^{(N)}_1(t) \equiv \rho^{(N)}_1(\mathbf{x}_1,t) \) which, together with the corresponding initial condition \( \rho^{(N)}_{1(o)}(\mathbf{x}_1) \), are stochastic, i.e., they are: 1) smoothly differentiable, 2) strictly positive and 3) summable in the sense that the velocity- or phase-space moments for the same PDF \( \rho^{(N)}_1(t) \) exist which correspond either to arbitrary monomial functions of \( v_1 \) (or its components \( v_{1,i} \), for \( i = 1, 2, 3 \)) or to the entropy density \( \ln \rho^{(N)}_1(t_o) \) (thus yielding \( S(\rho^{(N)}_1(t_o)) \), namely the BS-entropy functional evaluated in terms of the initial PDF). In particular, the smoothness and strict positivity conditions require that \( \rho^{(N)}_{1(o)}(\mathbf{x}_1) \) and \( \rho^{(N)}_1(t) \) are necessarily endowed with finite, i.e., non-zero, initial \( (L_\rho(t_o)) \) and global \( (L_\rho) \) characteristic scale-lengths, which are respectively defined as

\[
\begin{align*}
L_\rho(t_o) &= \inf_{\mathbf{x}_1 \in \Gamma_1} \left\{ \frac{\partial \ln \rho^{(N)}_1(\mathbf{x}_1,t)}{\partial \mathbf{r}_1} \right\}^{-1}, \\
L_\rho &= \inf_{(\mathbf{x}_1,t) \in \Gamma_1 \times I} \left\{ \frac{\partial \ln \rho^{(N)}_1(\mathbf{x}_1,t)}{\partial \mathbf{r}_1} \right\}^{-1}.
\end{align*}
\]

Given these premises we are now able to address the issues indicated above and in particular the inequality \( 33 \). Let us consider for this purpose an \( N \)-body hard-sphere system \( S_N \) such that in the continuum limit \( 33 \), for all \( N \equiv \frac{1}{\epsilon} \gg 1 \), the asymptotic ordering conditions

\[
\begin{align*}
N \sigma^2 &\sim O(\epsilon^0) \\
L_\rho &\sim O(\epsilon^0)
\end{align*}
\]

are fulfilled. Let us also assume that for arbitrary \( N \equiv \frac{1}{\epsilon} \gg 1 \) the dimensionless ratios \( \delta(t_o) \equiv \frac{\sigma}{\xi} \) and \( \delta \equiv \frac{\epsilon}{\xi} \) are similarly ordered requiring validity of one of the following initial and global "smoothness" ordering conditions, i.e., either (a) or (b), namely

\[
\begin{align*}
(a) \quad \delta(t_o) &\equiv \frac{\sigma}{\xi} \sim O(\epsilon^{1/2}) \\
(b) \quad \delta &\equiv \frac{\epsilon}{\xi} \sim O(\epsilon^{1/2}),
\end{align*}
\]

is fulfilled. Then for the global particular solutions indicated above which satisfy the global smoothness condition (b) the following propositions hold:

Proposition P\(_1\) \( \text{BG-limit of the 1-body occupation coefficient} \) - For all \( (\mathbf{r}_1,t) \in \Omega \times I \) the function \( k^{(N)}_1(\mathbf{r}_1,t) \) (see Eqs. [11]) admits the limit

\[
L_{BG}k^{(N)}_1(\mathbf{r}_1,t) = 1.
\]

Proposition P\(_2\) For all \( (\mathbf{r}_1,\ldots,\mathbf{r}_s,t) \in \Omega^s \times I \) and all \( s \geq 2 \) the \( s \)-body occupation coefficient \( k^{(N)}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s,t) \) (see Eq. [12]) admits the limit

\[
L_{BG}k^{(N)}_s(\mathbf{r}_1,\ldots,\mathbf{r}_s,t) = 1.
\]

Proposition P\(_3\) Denoting \( L_{BG}\rho^{(N)}_s(\mathbf{x}_1,\ldots,\mathbf{x}_s,t) \equiv \rho^{(N)}_s(\mathbf{x}_1,t) \) the \( 1 \)-body limit function PDF, for arbitrary \( s \geq 2 \) the limit function of the factorized \( s \)-body PDF \( 7 \) is provided by the summable PDF

\[
L_{BG}\rho^{(N)}_s(\mathbf{x}_1,\ldots,\mathbf{x}_s,t) = \prod_{i=1,s} \rho^{(N)}_1(\mathbf{x}_i,t),
\]

which is globally defined (for all \( t \in I \)) on the \( s \)-body phase space \( \Gamma^s \). The BG-limit is prescribed in the sense of uniform convergence of Cauchy sequences of smooth real scalar functions of \( \mathbf{x}, t \).

Proposition P\(_4\) \( \text{BG-limit of the Master equation} \) - In validity of the Master kinetic equation Eq. (13) the left \( \text{BG-limit} L_{BG}L_{1}\tilde{\rho}^{(N)}_1(\mathbf{x}_1,t) \) yields for all \( (\mathbf{x}_1,t) \in \Gamma_1 \times I \):

\[
L_{BG}L_{1}\tilde{\rho}^{(N)}_1(\mathbf{x}_1,t) = L_1 \rho^{(N)}_1(\mathbf{x}_1,t) - C_{1B}(\rho^{(N)}_1|\rho^{(N)}_1) = 0,
\]

where \( C_{1B}(\rho^{(N)}_1|\rho^{(N)}_1) \) is the usual BG-energy destruction term.
where $C_{1B}(\rho_1|\rho_1)$ denotes the Boltzmann collision operator

$$C_{1B}(\rho_1|\rho_1) = N \sigma^2 \int \, d\mathbf{v}_2 \int \, d\Sigma_{12} \left[ |\mathbf{v}_{12} \cdot \mathbf{n}_{12}| \left[ \rho_1(\mathbf{r}_1, \mathbf{v}_1^{(+)}, t) \rho_1(\mathbf{r}_1, \mathbf{v}_2^{(+)}, t) - \rho_1(\mathbf{r}_1, \mathbf{v}_1, t) \rho_1(\mathbf{r}_1, \mathbf{v}_2, t) \right] \right]$$

(see Ref. [23])

(24)

(see Ref. [23]) where

$$\int \, d\Sigma_{12}$$

(25)

denote the incoming (−) and outgoing (+)-particle sub-domain of solid angle where respectively $\mathbf{v}_{12} \cdot \mathbf{n}_{12} < 0$ or $\mathbf{v}_{12} \cdot \mathbf{n}_{12} > 0$. As a consequence the rhs thus of Eq. (23) coincides with the Boltzmann kinetic equation.

Proposition $P_3$ Right BG-limit of the Master equation - The right BG-limit $L_1 L_{BG}\hat{\rho}_1^{(N)}(x_1, t)$ yields instead on the same set

$$L_1 L_{BG}\hat{\rho}_1^{(N)}(x_1, t) = L_1 \rho_1(x_1, t),$$

(26)

so that necessarily for arbitrary 1-body PDFs fulfilling the smoothness conditions [19], the inequality [9] generally follows.

Let us outline here the proofs of propositions $P_1$ – $P_3$, details being left to the related references indicated below. To begin with, proposition $P_1$ follows as a consequence of the ordering assumptions [18] and (b) in Eq. [19]. Indeed one notices that by construction (i.e., again due to the same requirement (b) in Eq. [19]) both $\rho_1^{(N)}(x_1, t)$ and $k_1^{(N)}(r_1, t)$ are globally (i.e., for all $t \in I$) smoothly differentiable with respect to the position vector $r_1$. This implies in particular, denoting by $n_{21}$ a constant unit vector and upon considering $\varepsilon \ll 1$, that Taylor expansions with respect to $\varepsilon^{1/2}$ deliver

$$\left\{ \begin{array}{ll}
\hat{\rho}_1^{(N)}(\mathbf{r}_1 + \sigma \mathbf{n}_{21}, \mathbf{v}_1, t) = \rho_1^{(N)}(\mathbf{r}_1, \mathbf{v}_1, t) \left[ 1 + O(\varepsilon^{1/2}) \right], \\
\hat{k}_1^{(N)}(\mathbf{r}_1, \mathbf{v}_1, t) = k_1^{(N)}(\mathbf{r}_1, t) \left[ 1 + O(\varepsilon^{1/2}) \right].
\end{array} \right.$$  

(27)

Furthermore, one can show that under the same assumptions, arbitrary particular solutions of the Master kinetic equation $\rho_1^{(N)}(x_1, t)$ and the corresponding 1-body occupation coefficient $k_1^{(N)}(r_1, t)$ can be globally represented, respectively in the sets $\Gamma_1 \times I$ and $\Omega \times I$, in terms of first-order Taylor formulae with respect to $\varepsilon^{1/2}$, which take the form (see also Ref. [23])

$$\left\{ \begin{array}{ll}
\hat{\rho}_1^{(N)}(x_1, t) = \rho_1(x_1, t) + \Delta \rho_1(x_1, t; \varepsilon^{1/2}), \\
k_1^{(N)}(r_1, t) = 1 + \Delta r_1(r_1; \varepsilon^{1/2}).
\end{array} \right.$$  

(28)

Here $\rho_1(x_1, t)$ denotes a smooth PDF independent of $\varepsilon$, with $\Delta \rho_1(x_1, t; \varepsilon^{1/2})$ and $\Delta r_1(r_1; \varepsilon^{1/2})$ being the corresponding Taylor remainder-functions which are of order $O(\varepsilon^{1/2})$ and hence by construction vanish identically in the continuum limit [3].

The proof of $P_2$, i.e., that Eq. (21) is identically fulfilled, is analogous. It follows, besides the validity of proposition $P_1$, thanks to the factorization property of the $N$-body PDF (i.e., Eq. (4)) and the fact that, as a result, the appropriate integrals prescribed on infinite-dimensional domains necessarily must exist [36, 37].

Regarding $P_3$, its proof is an immediate consequence of the $s$-body factorized representation [8] and of propositions $P_1$ and $P_2$. Hence, the chaos property realized by Eq. (22) is satisfied identically in the extended phase space $\Gamma^s \times I$. Notice also that, thanks to the assumption of MCBC (see Eq. (6)), for all with $s \geq 2$ the existence of the factorized $s$-body limit functions [22] (usually referred to as “chaos property”), is warranted everywhere in the corresponding extended phase space $\Gamma^s \times I$. In contrast, adopting the PDF-conserving boundary condition (1) the same chaos property is always necessarily violated in a suitable subset of zero measure identifying the state after collision [19]. Thus, the crucial consequence of the "ab initio" theory is that, unlike Boltzmann’s and Grad’s approaches, for the prescription of the limit operator $L_{BG}$ convergence can be intended in the sense of Cauchy sequences, namely to apply everywhere in the corresponding extended phase-space. In fact, for arbitrary $s \geq 2$ in the BG-limit the $s$-body correlation functions $\Delta \rho_1^{(N)}(x_1, ..., x_s, t)$, which are prescribed according to Eq. (1), thanks to propositions $P_1$ and $P_2$ are given by

$$L_{BG} \Delta \rho_1^{(N)} = 0,$$  

(29)

i.e., consistent with Eq. (22), they indeed vanish identically in the same set $\Gamma^s \times I$.

Let us not consider proposition $P_4$. The proof of Eq. (23) is achieved in two steps. The first one is obtained by direct differentiation term by term in Eq. (13). Thus, evaluation of the differential operator $L_1 k_1^{(N)}(r_1, t)$ yields

$$L_1 k_1^{(N)}(r_1, t) = (N - 1) \int \frac{d\mathbf{x}_2 \cdot \mathbf{n}_{12} \times}{\Gamma_2} \delta(\mathbf{r}_1 - \mathbf{r}_2 - \sigma) \rho_1^{(N)}(\mathbf{x}_2, t) k_2^{(N)}(\mathbf{r}_1, \mathbf{r}_2, t) \mathcal{F}_2(\mathbf{r}).$$  

(30)

Hence, by substituting this identity in Eq. (13) and invoking MCBC, the same equation yields

$$L_1 \rho_1^{(N)}(x_1, t) = C_1 \left( \rho_1^{(N)} \right) \left( \rho_1^{(N)} \right).$$  

(31)

This identifies the second form of the Master kinetic
equation first introduced in Ref. [28]. In particular
\[ C_1 \left( \rho_1^{(N)} \left| \tilde{\rho}_1^{(N)} \right. \right) = (N - 1) \int d\nu_2 \int d\Sigma_{12} \]
\[ |v_{12} \cdot n_{12}| \sigma_{2}(\mathbf{r}) \tilde{\rho}_2^{(N)}(\mathbf{r}_1, v_1^{(+)}, \mathbf{r}_1 + \sigma n_{21}, v_2^{(+)}, t) - \]
\[ \tilde{\rho}_2^{(N)}(\mathbf{r}_1, v_1, \mathbf{r}_1 + \sigma n_{21}, v_2, t) \] (32)
denotes the corresponding Master collision operator. Notice here that, consistent with the causality principle [28, 29] but in contrast with the Boltzmann collision operator [24], the solid angle integration is performed in terms of the incoming particle subset prescribed according to Eq. (24). Next, based on Eq. (31), the second step of the proof involves taking into account the ordering assumptions (a) and (b) in Eq. (19), the power-series expansions (28) as well as propositions P1 and P2. As a consequence, consistent with the asymptotic estimates determined in Ref. [33], it is immediate to show that in the continuum limit (3) the following two identities hold
\[ \left\{ \begin{array}{l}
\mathcal{L}_{BG} L_{11} \rho_1^{(N)}(\mathbf{x}_1, t) = L_{1} \rho_1(\mathbf{x}_1, t), \\
\mathcal{L}_{BG} C_1 \left( \rho_1^{(N)} \right) = C_{1B} (\rho_1 | \rho_1),
\end{array} \right. \] (33)
with \( C_{1B} (\rho_1 | \rho_1) \) now denoting the customary form of the Boltzmann collision operator recalled above (see Eq. (24)). Notice, however, that here a key conceptual difference exists. In fact and in agreement with Ref. [28], but in contrast with the customary treatment of the Boltzmann collision integral the solid-angle integration can be equivalently carried out, thanks to MCBC, either w.r. to the incoming or outgoing particle subsets, i.e., respectively in terms of the corresponding solid-angle integrals [28] corresponding to the labels (−) or (+). Hence the Master equation, equivalently either in the first (19) or second (31) form, recovers exactly the Boltzmann equation (24).

Finally the proof of proposition P3 follows again thanks to P1, by noting that \( \mathcal{L}_{BG} \rho_1^{(N)}(\mathbf{x}_1, t) = \rho_1(\mathbf{x}_1, t) \) and \( \mathcal{L}_{BG} \rho_1^{(N)}(\mathbf{r}_1, t) = 1 \). This yields therefore the identity
\[ \mathcal{L}_{BG} \rho_1^{(N)}(\mathbf{x}_1, t) = \rho_1(\mathbf{x}_1, t), \] (34)
in turn implying at once Eq. (20), which provides the proof of the non-commutativity condition [5].

The immediate consequence of propositions P1 – P3 refers to the non-commutative property of the BG-operator \( \mathcal{L}_{BG} \) [5], implying that only the left BG-limits of the Master kinetic equation matters. This completes also the required prescription for \( \mathcal{L}_{BG} \) needed for the construction of the Boltzmann equation. In fact, the form of the resulting limit equation remains in principle non-unique, its precise realization depending critically on the way the action of the same operator is prescribed. As shown here this requires applying the BG-operator to the Master kinetic equation itself, i.e., evaluating the so-called left BG-limit of the same equation (rather than the right one), which yields identically the Boltzmann equation.

This conclusion appears relevant for the physical applications of the “ab initio” axiomatic approach to CSM, showing that the Master kinetic equation represents a solid basis for the establishment of kinetic theory and the investigation of granular, either dense or rarefied, hard-sphere particle systems.

However, a further remarkable development emerges. This concerns the establishment of global validity of the Boltzmann kinetic equation itself, a crucial problem also for its physical implications. Such a result is implied: 1) First, by the global validity of the Master kinetic equation, i.e., the global existence for all \((\mathbf{x}_1, t) \in \Gamma_1 \times I\) of stochastic 1-body PDFs which realize particular solutions of the same equation [32]; 2) Second, by the assumed validity of the asymptotic ordering requirement [18] and the global smoothness ordering condition (b) in Eqs. (19). Such a requirement provides in fact a sufficient condition for global validity of the Boltzmann equation. Indeed, as shown above it warrants, besides the Taylor expansions (28), the fact that the limit equation here determined (see Eq. (20)) coincides globally with the Boltzmann equation.

Nevertheless, the global validity problem remains still unsolved if the same assumption (b) is replaced with the initial smoothness ordering condition (a) (see again Eqs. (19)). The latter might actually not be sufficient to warrant global validity of the Boltzmann equation. In other words the question arises whether or under what initial conditions, related also to the occurrence of the phenomenon of decay to kinetic equilibrium for the Master kinetic equation [34], the ordering (b) in Eqs. (19) might be satisfied/violated in the same limit by arbitrary initial 1-body PDFs \( \rho_1^{(N)}(\mathbf{x}_1) \equiv \rho_1(\mathbf{x}_1) \) which are similarly smooth and prescribed so that \( \mathcal{L}_{BG}(t_o) \sim \mathcal{L}_{o} \sim O(\varepsilon^n) \).

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References

[1] L. Boltzmann, Wiener Berichte 66, 275 (1872).
[2] H. Grad, Handbook der Physik XII, 205 (1958).
[3] G.R. McNamara and G. Zanetti, Phys. Rev. Lett. 61, 2332 (1988).
[4] S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond (Numerical Mathematics and Scientific Computation), Oxford Science Publications (2001).
[5] R. A. Gingold J. J. Monaghan, Mon. Not. R. Astron. Soc. 181 (3): 375-389 (1977).
[6] S. Chapman and T. Cowling, The Mathematical Theory of Nonuniform Gases, Cambridge University Press (1951).
[7] C. Bardos, F. Golse and D. Levermore, J. Stat. Phys., 63(1-2), pp. 323-344 (1991).
[8] J. Loschmidt, Akademie der Wissenschaften zu Wien 73,128 (1876).
[9] E. Zermelo, Ann. d. Phys. 57, 485 (1896).
[10] L. Boltzmann, Wien. Ber. 66, 275 (1877); in Boltzmann Vol.II, pp. 112–148 (1909).
[11] J.L. Lebowitz, Phys. Today, November 1994, 115 (1994).
[12] C. Cercignani, Arch. Mech. 34, 231 (1982).
[13] A. Drory, S. Hist. Phil. Mod. Physics 39, 889 (2008).
[14] J. Uffink, G. Valente, Found Phys. 45,404 (2015).
[15] Massimo Tessarotto, Claudio Cremaschini and Marco Tessarotto, Eur. Phys. J. Plus 128, 32 (2013).
[16] D. Enskog, Kungl. Svensk Vetenskps Akademiens 63, 4 (1921); (English translation by S. G. Brush, Kinetic Theory, Vol. 3, Pergamon, New York, 1972).
[17] C. Cercignani, Theory and applications of the Boltzmann equation, Scottish Academic Press, Edinburgh and London, p. 48 Eq. (2.14) (1975).
[18] L. Boltzmann, Vorlesungen über Gasstheorie, 2 vol., J.A. Barth, Leipzig (1896-1898); English transl. by H. Brush, Lectures on gas theory, University of California Press, Vol. 1, Section 12 and Vol. 2, Section 22.
[19] C. Cercignani, 134 years of Boltzmann equation, p. 107 in Boltzmann’s legacy, (G. Gallavotti, W. Reiter and J. Yngvason Eds.), ESI Lecture in Mathematics and Physics, European Mathematical Society (2008).
[20] ibid, Vol. 1, Section 8.
[21] ibid, Vol. 2, Section 38.
[22] A. Munster, Statistical Thermodynamics, Springer (1969).
[23] O.E. Lanford, Time evolution of large classical systems, Lecture Notes in Physics, Vol.38 (Springer,Berlin, p.1 (1975).
[24] O.E. Lanford, Soc. Math. de France, Asterisque 40, 117 (1976).
[25] O.E. Lanford, Physica 106A, 70 (1981).
[26] C. Villani, Entropy production and convergence to equilibrium for the Boltzmann equation, 14th Int. Congress on Math. Physics (28 July-2 August 2003 Lisbon, Portugal), Ed. J.C. Zambrini (University of Lisbon, Portugal), published by World Scientific Publishing Co. (2006).
[27] M. Tessarotto and C. Cremaschini, Phys. Lett. A 378, 1760 (2014).
[28] M. Tessarotto and C. Cremaschini, Eur. Phys. J. Plus 129, 157 (2014).
[29] Massimo Tessarotto and C. Cremaschini, Eur. Phys. J. Plus 129, 243 (2014).
[30] M. Tessarotto and C. Cremaschini, Phys. Lett. A 379, 1206 (2015).
[31] M. Tessarotto and C. Cremaschini, Eur. Phys. J. Plus 130, 91 (2015).
[32] M. Tessarotto, C. Asci, C. Cremaschini, A. Soranzo and G. Tironi, Eur. Phys. J. Plus 130, 160 (2015).
[33] M. Tessarotto and C. Asci, Phys. Lett. A 381, 1484 (2017).
[34] M. Tessarotto, M. Mond and C. Asci, Eur. Phys. J. Plus 132, 213 (2017).
[35] C. Cercignani, Mathematical methods in kinetic theory, Plenum Press, New York (1969).
[36] C. Asci, Int. J. An., doi:org/10.1155/2014/ 404186 (2014).
[37] C. Asci, J. Math., doi:org/10.1155/2016/2619087 (2016).