Global validity of the Master kinetic equation for hard-sphere systems

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Following the recent establishment of an exact kinetic theory realized by the Master kinetic equation which describes the statistical behavior of the Boltzmann-Sinai Classical Dynamical System (CDS), in this paper the problem is posed of the construction of the related global existence and regularity theorems. For this purpose, based on the global prescription of the same CDS for arbitrary single and multiple collision events, first global existence is extablished for the $N-$body Liouville equation which is written in Lagrangian differential and integral forms. This permits to reach the proof of global existence both of generic $N-$body probability density functions (PDF) as well as of particular solutions which maximize the statistical Boltzmann-Shannon entropy and are factorized in terms of the corresponding $1-$body PDF. The latter PDF is shown to be uniquely defined and to satisfy the Master kinetic equation globally in the extended $1-$body phase space. Implications concerning the global validity of the asymptotic Boltzmann equation and Boltzmann H-theorem are discussed.

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1 - INTRODUCTION

In the present paper the problem is posed of investigating the global validity properties possibly associated with the Boltzmann-Sinai classical dynamical system (S_N-CDS) and its statistical description. The said CDS advances in time the Newtonian state $\mathbf{x} \equiv (\mathbf{r}, \mathbf{v}) \equiv \{\mathbf{x}_1, ..., \mathbf{x}_N\}$ of a closed and isolated set S_N of N smooth hard spheres, a model that is widely used in the literature for the description of real systems like granular gases as well as for mathematical investigations based on kinetic and/or statistical descriptions for systems of extended particles. The same particles are assumed to undergo both single and multiple elastic collisions which satisfy appropriate *collision laws* to be discussed in detail below (see Section 2). For definiteness, in this context each particle is described by a Newtonian state $\mathbf{x}_i = (\mathbf{r}_i, \mathbf{v}_i)$, represented by the center of mass position and velocity vectors $\mathbf{r}_i$ and $\mathbf{v}_i$, and is endowed with a mass m and a diameter σ. Here $\mathbf{x}$ and $\mathbf{x}_i$ span respectively the $N-$body phase-space $\Gamma_N = \prod_{i=1,N} \Gamma_{1(i)}$ and the $i-$th particle $1-$body phase-space $\Gamma_{1(i)} = \Omega_i \times V_i$, with $V_i \equiv \mathbb{R}^3$ and $\Omega_i \equiv \Omega \subset \mathbb{R}^3$ denoting the $i-$th particle velocity and configuration spaces. In particular Ω is identified with the bounded interior of a $3-$dimensional parallelepiped having a stationary and rigid boundary.

In our opinion the goal indicated above, besides present day mathematics, appears potentially of crucial importance in view of the investigation of time-asymptotic properties of the theory which are relevant for a wide range of related physical applications. This is based, in fact, on the new "ab initio" treatment of classical statistical mechanics (CSM), recently developed in Refs. [1–6], enabling the treatment of granular systems formed by a finite number of particles. Key feature of such an approach is that of permitting the adoption of an extended functional setting for the microscopic statistical description of the same S_N-CDS. The latter relies on the physical requirement that the $N-$body probability density function (PDF) $\rho^{(N)}(\mathbf{x},t)$ solution of the Γ_N-*phase-space Liouville equation*, by construction, should satisfy at arbitrary collision events appropriate *modified collision boundary conditions* (MCBC) [2]. The latter uniquely relate the incoming and outgoing $N-$body PDF, i.e., immediately before and after an arbitrary collision event. As a consequence, it is found that the $N-$body PDF now can include among its physically-admissible realizations both stochastic, partially deterministic and deterministic PDF [1, 3]. In addition, the same Γ_N-phase-space Liouville equation necessarily admits among its physically-admissible solutions also a permutation-symmetric, particular realization of the $N-$body PDF which is factorized in terms of the corresponding $1-$body PDFs $\rho_1^{(N)}(\mathbf{x}_i,t)$ for all $i = 1, N$. As recalled below (see also Refs. [3] and [6]), the really remarkable implication which follows is that the same $1-$body PDF $\rho_1^{(N)}(t) \equiv \rho_1^{(N)}(\mathbf{x}_1,t)$ satisfies an equivalent exact, i.e., non-asymptotic kinetic equation holding for finite values of (N, σ, m), denoted as *Master kinetic equation,* while in addition the corresponding Boltzmann-Shannon $1-$body entropy $S(\rho_1^{(N)}(t))$ (see definition below in Eq. (9)) is identically conserved for all $t \in I \equiv \mathbb{R}$ (*Master H-theorem*).

Here we intend to investigate two basic mutually-related issues. The first one deals with the conditions which permit the unique, i.e., deterministic, global prescription of the Boltzmann-Sinai CDS for arbitrary collision events.

The second issue concerns the identification of the most general conditions which warrant for the same S_N-CDS the existence of a global unique solution of the Γ_N-phase-space Liouville equation and in particular also of the Master kinetic equation and of the corresponding Master H-theorem. As an application, we intend also to highlight the main implications which apply to the Boltzmann equation and Boltzmann H-theorem, to be intended in such a framework, as in Ref. [6], just as a suitable asymptotic approximation of the same Master kinetic equation and Master H-theorem respectively.

Historical ante factum and motivations

Although Boltzmann's equation and Boltzmann H-Theorem [7–10] are 143 years old, certain aspects of their derivation have remained for a long time unsatisfactory. Two obvious issues in fact actually arise in this connection. The first one is whether a unique solution of the Boltzmann equation exists so that also the Boltzmann-Shannon statistical entropy $S_1(\rho_1(t))$ associated with the $1-$body PDF $\rho_1(t) \equiv \rho_1(\mathbf{x}_1, t)$ solution of the Boltzmann equation actually exists in a global sense, namely for all $t \in I$. Here the same functional is prescribed (actually up to the sign) according to the Boltzmann original definition, i.e., letting $S_1(\rho_1(t)) \equiv -\int\limits_{\Gamma_{1(1)}} d\mathbf{x}_1 \rho_1(\mathbf{x}_1, t) \ln \rho_1(\mathbf{x}_1, t)$. Such a definition, nevertheless, is consistent up to arbitrary multiplicative and additive constants with that reported below (see Eq. (9)). The second one is whether in such a case the limit

$$\lim_{t \to +\infty} S_1(\rho_1(t)) \tag{1}$$

exists too. A satisfactory answer to these issues does not exists yet, at least if one remains in the framework of the original Boltzmann approach. In fact according to the *Villani's disclaimer* [11]*: "... mathematics is unable to prove it rigorously and in satisfactory generality...* (the obstacle being that)*... we don't know whether solutions of the Boltzmann equation are smooth enough, except in certain particular cases (close-to-equilibrium theory, spatially homogeneous theory, close-to-vacuum theory)".* The current status remains to date essentially unchanged. In fact, global existence proofs provided more recently, such for example as in Ref. [12], do not overcome, despite contrary claims of the authors, the limitations stated above.

However additional, possibly even more serious, difficulties arise which are intrinsically related to the Boltzmann's original approach. To be able to identify them requires, however, changing the customary perspective taken usually in the prevailing mathematical literature [13] and to start, instead, from a first-principle approach based on the axioms of Classical Statistical Mechanics (CSM) applying in principle for an arbitrary $N-$body CDS. Indeed, according to Edwin Thompson Jaynes [14] this is the only route that can afford any serious advancement in such a context, and hence "*a fortiori*" regarding a better understanding of Boltzmann's kinetic theory itself. An axiomatic theory of this type, which actually should afford a thorough critical review of this type, has been recently developed based on the "*ab initio*" approach to CSM (see related the presentation given in Ref. [1], as well as Refs. [2, 3]).

One of the main obstacles, which emerges in this way, is actually the same one which is shared by many of the famous fundamental equations of mathematical physics: their asymptotic character. In the case of the Boltzmann kinetic equation this conclusion, which is actually inherent in its very construction method which requires the simultaneous validity of the so-called dilute-gas asymptotic ordering as well as of the Boltzmann-Grad limit [3–6], follows from compelling physical evidence. This is realized by the following basic physical issues arising in the context of Boltzmann kinetic theory, which concern:

- *Issue #1: functional setting of the Boltzmann equation.* As pointed out in Ref. [1] (see also Ref. [2]), distributions such as the *deterministic* $1-$*body PDF* which is realized by means of the $1-$body phase-space Dirac delta, namely for the $i-$th particle

$$\rho_{H1}^{(N)}(\mathbf{x}_i, t) = \delta\left(\mathbf{x}_i - \mathbf{x}_i(t)\right), \tag{2}$$

or analogous *partially-deterministic PDFs* of the type given in the Appendix (see Eq. (84)), are possibly ruled out from the class of admissible solutions for the same equation. This feature is in conflict with the basic principles of CSM. Indeed these require that *classical deterministic mechanics* (CDM) should be recovered as particular possible realization of CSM and hence of kinetic theory. As a consequence distributions of the type indicated above, and in particular the $N-$body phase-space Dirac delta should be included in the *class of admissible solutions* for CSM and hence correspondingly the $1-$body phase-space Dirac delta should pertain to kinetic theory as well.

- *Issue #2: violation of the Boltzmann equation and related Boltzmann H-theorem.* A first consequence which logically follows from *issue #1* is that for distributions of the type indicated above, and in particular in case of the $1-$body deterministic PDF, both the Boltzmann equation and the related Boltzmann H-theorem are actually *patently violated.*

- *Issue #3: violation of the collision boundary conditions (CBC).* In the literature starting from Boltzmann original approach [7] (see for related discussion in Ref. [17]) the dynamical evolution of the $N-$body PDF $\rho^{(N)}(\mathbf{x},t)$ across arbitrary collision events is realized by the causal equation

$$\rho^{(-)(N)}(\mathbf{x}^{(-)}(t_i),t_i) = \rho^{(+)(N)}(\mathbf{x}^{(+)}(t_i),t_i), \tag{3}$$

to be referred to as *PDF-conserving collision boundary condition* (CBC). Here $\rho^{(\pm)(N)}(\mathbf{x}^{(\pm)}(t_i),t_i) = \lim_{t\to t_i^{(\pm)}} \rho^{(N)}(\mathbf{x}(t),t)$ denote for $(-)$ and $(+)$ the incoming and outgoing PDFs ($\rho^{(-)(N)}$ and $\rho^{(+)(N)}$), which are here expressed respectively in terms of the corresponding incoming and outgoing states $\mathbf{x}^{(-)}(t_i)$, and $\mathbf{x}^{(+)}(t_i)$, which are defined as

$$\mathbf{x}^{(\pm)}(t_i) = \lim_{t\to t_i^{(\pm)}} \mathbf{x}(t). \tag{4}$$

In particular, invoking the property of left continuity at all collision times $\rho^{(-)(N)}(\mathbf{x}^{(-)}(t_i),t_i)$ on the lhs of Eq. (3) can be replaced with $\rho^{(N)}(\mathbf{x}^{(-)}(t_i),t_i)$. Notice that the relationship between the states $\mathbf{x}^{(+)}(t_i)$ and $\mathbf{x}^{(-)}(t_i)$ is determined by the collision laws occurring for hard spheres (see discussion below in Section 3). As shown in Ref. [2] the PDF-conserving CBC (3) is incompatible with the existence of the $N-$body deterministic PDF. Hence it is physically inconsistent with the extended functional setting indicated *issue #1.*

- *Issue #4: physical consistency of the Boltzmann-Grad limit.* A final basic issues must be mentioned, which concerns the physical consistency of the Boltzmann-Grad limit adopted in the original Boltzmann's approach (see also [25–29]). In this regard, since Enskog and Chapman and Enskog contributions [15, 16], it is well-known that the Boltzmann-Grad limit becomes intrinsically invalid for statistical treatment of locally dense or dense gases as well as for granular fluids, i.e., in which hard-spheres are assumed as finite-size (see related discussions in Refs. [1, 3]). Nevertheless, from the physical standpoint the Boltzmann-Grad limit "*per se*" just makes no sense even for dilute gases. In fact, the number N of physical molecules contained, for example, in a (gas or fluid) mole must remain necessarily finite (indeed, in such a case N may be identified with the Avogadro number). There is clear evidence that Boltzmann himself was aware of the potential contradiction between real physical molecular systems and his mathematical hard-sphere model. In this regard, it is instructive to read also the related discussion reported in Cercignani's last review paper on Boltzmann equation [19]. In fact, while acknowledging the finiteness of the *physical* values of N and ε, Boltzmann clearly considered the adoption of the Boltzmann-Grad limit as a requirement for his mathematical model. In particular, according to own Boltzmann's statement, such a limit is a prerequisite for the validity of the stosszahlansatz condition, and hence for the construction of the Boltzmann kinetic equation and the subsequent derivation of the related H-theorem. In this regard, a basic issue is therefore whether, consistent with physical requirements, the asymptotic limit $N\to\infty$ can actually be replaced by the weaker asymptotic condition $N \gg 1$ or even $N \sim 1$ in order to achieve a kinetic description of the hard sphere system S_N-CDS in the context of an axiomatic approach.

Goals of the investigation

In this paper we intend to address the problem of global validity for the statistical description of the Boltzmann-Sinai CDS. This is based on the "*ab initio*" treatment of classical statistical mechanics which holds for a system of smooth hard spheres characterized by finite values of the parameters (N,m,σ) [1–6]. More precisely, we intend to show that, once the same CDS has been uniquely globally prescribed, global existence and uniqueness for the Master kinetic equation, to be established in the framework of the extended functional setting recalled above, follow as an elementary consequence of the global existence and uniqueness property for the corresponding Γ_N-phase-space Liouville equation as well as the determination for the latter of the $N-$body factorized extremal PDF.

Finally, in view of the relationship recalled above between the Master and Boltzmann kinetic equations holding in the asymptotic dilute-gas approximation, the problem is posed of establishing possible conditions for the existence of global solutions for the Boltzmann equation too. In the light of such considerations in the sequel the following goals are pursued:

- *GOAL #1: Unique global prescription of the Boltzmann-Sinai classical dynamical system S_N-CDS.*
- *GOAL #2: Global unique prescription of the $N-$body PDF generic solution of the Γ_N-phase-space Liouville equation*
- *GOAL #3: Global unique prescription of the $N-$body PDF factorized solution of the Γ_N-phase-space Liouville equation*
- *GOAL #4: Global unique prescription of the $1-$body PDF solution of the Master kinetic equation*
- *GOAL #5: Analysis of the implications of Goals #1-#4 on the Boltzmann kinetic equation and Boltzmann H-theorem.*

2 - THE EMERGING NEW "AB INITIO" APPROACH

Despite the fundamental nature of the physical considerations therein involved and the consequent possible mathematical implications, the very existence of the *issues #1-#4* indicated above has apparently gone unnoticed in the past literature, with the possible exception of the last one. Nevertheless it must be noted that neither Boltzmann himself, nor anybody else after him, as far as we know, ever succeeded in dealing with the matter. The solution of the previous issues lays at the basis of the new statistical approach recently developed [1–3]. This is based, in particular, on two key requirements.

The first one concerns the introduction, pointed out in Refs. [1–3], of an extended functional setting prescribing the functional class of the admissible $N-$body PDF $\rho^{(N)}(t) \equiv \rho^{(N)}(\mathbf{x},t)$ solutions of the Γ_N-phase-space Liouville equation for the S_N-CDS. More precisely, $\rho^{(N)}(\mathbf{x},t)$ is identified either with a generic stochastic PDF or coincides with a suitable kind of distribution (see definitions recalled for greater clarity in the Appendix). As shown in Refs. [1–3], the extended functional setting involves also the adoption on the collision subset $\delta\Gamma_N$ (see definition in the Appendix) of a new type of CBC for the N $-$body PDF which differ from the PDF-conserving CBC recalled above (see Eq. (3)) previously adopted in the literature and usually ascribed to Boltzmann himself [7] (see also for example Ref. [17]). The new prescription, denoted as *modified collision boundary conditions* (MCBC), has been found to be a mandatory requirement, based on purely physical grounds, i.e., the "*ab initio*" approach for the statistical treatment of the S_N-CDS developed in Ref. [1]. In fact, it is needed for the validity of CSM [1] when the deterministic $N-$body PDF is included in the functional class of the admissible $N-$body PDFs. In the admissible subset $\widehat{\Gamma}_N$ it takes the equivalent form

$$\rho_H^{(N)}(\mathbf{x},t) = \delta\left(\mathbf{x}-\mathbf{x}(t)\right) \equiv \prod_{i=1,N} \rho_{H1}^{(N)}(\mathbf{x}_i,t), \tag{5}$$

with $\delta\left(\mathbf{x}-\mathbf{x}(t)\right)$ denoting the $N-$body Dirac-delta function and $\rho_{H1}^{(N)}(\mathbf{x}_i,t)$ the $i-$th particle $1-$body deterministic PDF given by Eq. (2). This condition follows as a consequence of the assumption that CSM must recover classical deterministic mechanics as one of its (infinite) possible realizations. Due to such an overriding constraint, in Refs. [1, 2] it was shown that CBC must actually be identified with MCBC. For definiteness, let us denote respectively the outgoing and incoming PDFs $\rho^{(-)(N)}(\mathbf{x}^{(-)}(t_i),t_i)$ and $\rho^{(+)(N)}(\mathbf{x}^{(+)}(t_i),t_i)$, with $\rho^{(\pm)(N)}(\mathbf{x}^{(\pm)}(t_i),t_i) = \lim_{t\to t_i^{(\pm)}} \rho^{(N)}(\mathbf{x}(t),t)$, where $\mathbf{x}^{(-)}(t_i)$ and $\mathbf{x}^{(+)}(t_i)$, with $\mathbf{x}^{(\pm)}(t_i) = \lim_{t\to t_i^{(\pm)}} \mathbf{x}(t)$, are the incoming and outgoing Lagrangian $N-$body states, their mutual relationship being again determined by the collision laws holding for the S_N-CDS (see again Section 3). For an arbitrary $N-$body PDF $\rho^{(N)}(\mathbf{x},t)$ belonging to the extended functional setting and an arbitrary collision event occurring at time t_i two possible realizations the MCBC can in principle be given, both yielding a relationship between the PDFs $\rho^{(+)(N)}$ and $\rho^{(-)(N)}$. These are provided by the two MCBC expressed in Lagrangian form and realized respectively either by

$$\rho^{(+)(N)}(\mathbf{x}^{(+)}(t_i),t_i)=\rho^{(-)(N)}(\mathbf{x}^{(+)}(t_i),t_i), \tag{6}$$

or

$$\rho^{(-)(N)}(\mathbf{x}^{(-)}(t_i),t_i)=\rho^{(+)(N)}(\mathbf{x}^{(-)}(t_i),t_i). \tag{7}$$

Once the time-axis is oriented, i.e., the arrow of time is prescribed, it follows that Eq. (6) predicts the future (i.e.,outgoing) PDF from the past (incoming) one. Hence the choice (6) is the one which is manifestly consistent with the causality principle. The causal Eulerian form of MCBC corresponding to Eq. (6) is then provided by the condition

$$\rho^{(+)(N)}(\mathbf{x}^{(+)},t)=\rho^{(-)(N)}(\mathbf{x}^{(+)},t), \tag{8}$$

where now $\mathbf{x}^{(+)}$ denotes again an arbitrary outgoing collision state. It must be stressed that the modified boundary conditions indicated above radically depart from the customary ones adopted in the literature (see Ref. [17]), namely the PDF-conserving CBC (3) given above (see related discussions in Refs. [1, 2]).

Theoretical aspects of the new "ab initio " approach have previously been discussed in detail in a series of papers (see Refs. [3–6]). The consequences are widespread. They concern a number of important new achievements in CSM and kinetic theory, which are the basis of the subsequent discussion on global existence. In particular they include:

- *Result #1: Maximal form of the principle of entropy maximization (PEM).* As discussed in Ref. [3] the role and the consequences of the Principle of entropy maximization (PEM [32, 33]) and the notion of $s-$body Boltzmann-Shannon (BS) entropy (for $s=1,N$) to be adopted for the statistical description of the S_N-CDS have been analyzed. As shown in Refs. [1, 6] for an arbitrary stochastic $s-$body PDF $\rho_s^{(N)}(t)\equiv\rho_s^{(N)}(\mathbf{x}^{(s)},t)\equiv F_s\left\{\rho^{(N)}(\mathbf{x},t)\right\}$, with $\mathbf{x}^{(s)}=\{\mathbf{x}_1,...,\mathbf{x}_s\}$ and F_s a suitable integral operator (see Eq. (16) below), this is given for all $s=1,N$ by

$$S_s(\rho_s^{(N)}(t))=-\alpha_s^2\int\limits_{\Gamma_s}d\mathbf{x}^{(s)}\rho_s^{(N)}(\mathbf{x}^{(s)},t)\ln\frac{\rho_s^{(N)}(\mathbf{x}^{(s)},t)}{A_s}, \tag{9}$$

  with $\alpha_s,A_s\in\mathbb{R}$ arbitrary constants such that $\alpha_s\neq 0$ and $A_s>0$. Indeed, based on the "maximal form" of PEM, namely the requirement that a prescribed initial time $t_o\in I$ all $s-$body BS entropies have the same maximal initial value, the extremal initial $N-$body PDF $\rho^{(N)}(\mathbf{x},t_o)$ is found to be uniquely factorized in terms of the 1$-$body PDF. For definiteness, let us consider the admissible subset of Γ_N formed by all accessible states (see Appendix). Then in such a set $\rho^{(N)}(\mathbf{x},t_o)$ necessarily takes the form:

$$\begin{aligned}\rho^{(N)}(\mathbf{x},t_o) &= \widehat{\rho}^{(N)}(\mathbf{x},t_o),\\ \widehat{\rho}^{(N)}(\mathbf{x},t_o. &\equiv \prod_{i=1,N}\frac{\widehat{\rho}_1^{(N)}(\mathbf{x}_i,t_o)}{k_1^{(N)}(\mathbf{r}_i,t_o)},\end{aligned} \tag{10}$$

  with $\rho_1^{(N)}(\mathbf{x}_i,t_o)\equiv\rho_1^{(N)}(\mathbf{x}_i,t_o)$ and $k_1^{(N)}(\mathbf{r}_i,t_o)$ denoting the 1$-$body occupation coefficient defined below (see Eq. (14)). The $N-$body PDF, if it exists, which for arbitrary $t\in I$ corresponds to the initial condition (10) will be referred to here as the *$N-$body factorized extremal PDF.*

- *Result #2: Construction of an exact kinetic equation, denoted as Master kinetic equation.* As shown in Ref. [3] the statistical treatment of the S_N-CDS based on "*ab initio*" approach permits to reach an exact kinetic equation for the corresponding 1$-$body PDF. Its explicit realization is as follows

$$L_{1(1)}\rho_1^{(N)}(\mathbf{x}_1,t)=\mathcal{C}_1\left(\rho_1^{(N)}|\rho_1^{(N)}\right), \tag{11}$$

  where $L_{1(1)}=\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\frac{\partial}{\partial\mathbf{r}_1}$ is the 1$-$body free-streaming operator and where $\mathcal{C}_1\left(\rho_1^{(N)}|\rho_1^{(N)}\right)$, denoted as Master collision operator, is given by

$$\mathcal{C}_1\left(\rho_1^{(N)}|\rho_1^{(N)}\right)\equiv(N-s)\,\sigma^2\int\limits_{U_{1(2)}}d\mathbf{v}_2\int^{(-)}d\Sigma_{21}\left[\widehat{\rho}_2^{(N)}(\mathbf{x}^{(2)(+)},t)-\widehat{\rho}_2^{(N)}(\mathbf{x}^{(2)},t)\right]|\mathbf{v}_{21}\cdot\mathbf{n}_{21}|\,\overline{\Theta}^*. \tag{12}$$

Here $\overline{\Theta}^{*}\equiv\overline{\Theta}\left(\left|\mathbf{r}_{2}=\mathbf{r}_{1}+\sigma\mathbf{n}_{21}-\frac{\sigma}{2}\mathbf{n}_{2}\right|-\frac{\sigma}{2}\right)$, while $\widehat{\rho}_{2}^{(N)}(\mathbf{x}^{(2)(+)},t)$ denotes the outgoing 2−body PDF

$$\widehat{\rho}_{2}^{(N)}(\mathbf{x}^{(2)(+)},t)\equiv\frac{k_{2}^{(N)}(\mathbf{r}_{1},\mathbf{r}_{2},t)}{k_{1}^{(N)}(\mathbf{r}_{1},t)k_{1}^{(N)}(\mathbf{r}_{2},t)}\rho_{1}^{(N)}(\mathbf{r}_{1},\mathbf{v}_{1}^{(+)},t)\rho_{1}^{(N)}(\mathbf{r}_{2},\mathbf{v}_{2}^{(+)},t),\tag{13}$$

in which $\mathbf{r}_{2}$ is identified with $\mathbf{r}_{2}=\mathbf{r}_{1}+\sigma\mathbf{n}_{21}$ and the integral in Eq. (12) is evaluated on the subset in which $\mathbf{v}_{12}\cdot\mathbf{n}_{12}<0$. Furthermore, $k_{2}^{(N)}(\mathbf{r}_{1},\mathbf{r}_{2},t)$ identify the 2-body occupation coefficients. As shown in Ref. [3] the form of both $k_{1}^{(N)}(\mathbf{r}_{i},t)$ and $k_{2}^{(N)}(\mathbf{r}_{1},\mathbf{r}_{2},t)$ is uniquely prescribed by the 1−body PDF. More precisely they are determined by means of the integral equations

$$k_{1}^{(N)}(\mathbf{r}_{1},t)\equiv F_{1}\left\{\prod_{j=2,N}\frac{\rho_{1}^{(N)}(\mathbf{x}_{j},t)}{k_{1}^{(N)}(\mathbf{r}_{j},t)}\right\},\tag{14}$$

$$k_{2}^{(N)}(\mathbf{r}_{1},\mathbf{r}_{2},t)\equiv F_{2}\left\{\prod_{j=s+1,N}\frac{\rho_{1}^{(N)}(\mathbf{x}_{j},t)}{k_{1}^{(N)}(\mathbf{r}_{j},t)}\right\},\tag{15}$$

where F_s is the integral operator

$$F_{s}\equiv\int_{\Gamma_{N}}d\overline{\mathbf{x}}\Theta^{(N)}(\overline{\mathbf{r}})\prod_{i=1,s}\delta(\mathbf{x}_{i}-\overline{\mathbf{x}}_{i}).\tag{16}$$

The fundamental novelty of the Master equation, which sets it apart from previous literature, lies in the adoption of MCBC. The equation exhibits a number of physically-relevant properties. First, it is indeed in a proper sense a kinetic equation, since it depends functionally only on the same 1−body PDF.

Second, it admits both stochastic and deterministic or partially-deterministic 1−body PDFs (see Eq. (2)) among its admissible particular realizations, so that in principle it is suitable for the treatment of both dense and rarefied granular fluids. A notable difference with respect to the Boltzmann equation is that the Master equation is non-asymptotic, in the sense that it holds without imposing approximations or asymptotic conditions on the underlying CDS. As a consequence the S_N−CDS is defined only provided the parameters N and σ are both considered as finite, namely such that $N<\infty$ and $\sigma>0$ respectively [1]. Nevertheless, the same parameters N and σ can still satisfy suitable asymptotic orderings, which correspond to precise configurations of physical interest. In the following we shall refer in particular to the so-called *dilute gas* (or rarefied gas) *asymptotic ordering* obtained by prescribing at the same time

$$\begin{aligned}N&\equiv\frac{1}{\varepsilon}\gg1,\\0&<\sigma\sim O(\varepsilon^{1/2}),\end{aligned}\tag{17}$$

namely that the Knudsen number $K_n\equiv N\sigma^2$ becomes of $O(\varepsilon^0)$. Hence, the Master kinetic equation realizes a rigorous statistical treatment of the molecular dynamics occurring in these systems for arbitrary finite values of N and σ also in the sense indicated above.

- *Result #3: Determination of a constant H-theorem.* As pointed out in Ref. [6] the Master kinetic equation admits a constant H-theorem. More precisely, let us assume that $\rho_{1}^{(N)}(t_o)\equiv\rho_{1}^{(N)}(\mathbf{r}_{1},\mathbf{v}_{1},t_o)$ is an arbitrary stochastic 1−body PDF solution of the Master kinetic equation which satisfies the initial condition

$$\rho_{1}^{(N)}(\mathbf{r}_{1},\mathbf{v}_{1},t_o)=\rho_{1o}^{(N)}(\mathbf{r}_{1},\mathbf{v}_{1})\tag{18}$$

and admits the Boltzmann-Shannon entropy $S_1(\rho_{1}^{(N)}(t_o))$. Then for all $t\in I$ for which $\rho_{1}^{(N)}(\mathbf{r}_{1},\mathbf{v}_{1},t)$ exists

$$S_1(\rho_{1}^{(N)}(t))=S_1(\rho_{1}^{(N)}(t_o)),\tag{19}$$

i.e., the Boltzmann-Shannon entropy $S_1(\rho_{1}^{(N)}(t))$ is conserved (*Master H-theorem*).

- *Result #4: Derivation of the Boltzmann kinetic equation in terms of the Master kinetic equation.* In Ref. [3] the Boltzmann equation was shown to follow from the Master equation by invoking the Boltzmann-Grad limit. However the same equation can also be recovered in an asymptotic sense when the so-called *dilute-gas asymptotic approximation* is introduced in the Master kinetic equation (see also Ref. [4]) This involves, as discussed in Ref. [6], besides the validity of the asymptotic ordering (17) the validity of suitable approximations for the 1$-$ and 2$-$body PDF which are recalled below (see Section 7).

- *Result #5: Derivation of Boltzmann H-theorem from the Master H-theorem.* As shown in Ref. [6], upon invoking the dilute-gas asymptotic approximation indicated above for the 1$-$body PDF one obtains

$$S_1(\rho_1^{(N)}(t)) = S_1(\rho_1(t))\left[1 + O\left(\varepsilon^{1/2}\right)\right] \tag{20}$$

where on the rhs $S_1(\rho_1(t))$ denotes the Boltzmann-Shannon entropy associated with the 1$-$body PDF solution of the Boltzmann kinetic equation. Then, as proved in Ref. [6], consistent with Boltzmann H-theorem, it follows necessarily that

$$\frac{\partial}{\partial t} S_1(\rho_1(t)) \geq 0. \tag{21}$$

3 - GLOBAL UNIQUE PRESCRIPTION OF THE BOLTZMANN-SINAI CDS

Let us first notice that the Boltzmann-Sinai S_N-CDS is globally defined and time-reversible, if it realizes for all $t \in I$ a uniquely-prescribed bijection on the $N-$body phase-space Γ_N, i.e., of the form

$$\mathbf{x}(t_o) \equiv \mathbf{x}_o \rightarrow \mathbf{x}(t) \equiv \chi(\mathbf{x}_o, t_o, t), \tag{22}$$

with inverse

$$\mathbf{x}(t) \equiv \mathbf{x} \rightarrow \mathbf{x}(t_o) \equiv \chi(\mathbf{x}, t, t_o), \tag{23}$$

where for all $t, t_o \in I$, $\chi(\mathbf{x}_o, t_o, t)$ is a real and autonomous vector field, i.e., of the type

$$\chi(\mathbf{x}_o, t_o, t) = \chi(\mathbf{x}_o, \tau), \tag{24}$$

with $\tau \equiv t - t_o$. As a "*sine qua non*" requirement needed **to** define S_N-CDS, the collision laws for hard-sphere collisions referred to above must be uniquely and globally prescribed, with definitions independent of space and time. At an arbitrary collision time $t_i \in \{t_i\}$, i.e., in which one or more particles are in simultaneous contact with each other and/or with the boundary, while being endowed with non-vanishing relative velocities, the collision laws are therefore functions of the incoming and outgoing states $\mathbf{x}^{(-)}(t_i)$, and $\mathbf{x}^{(+)}(t_i)$ (see Eq. (12)). Hence, they are necessarily of the form

$$\mathbf{x}^{(-)}(t_i) \rightarrow \mathbf{x}^{(+)}(t_i) \equiv \chi(\mathbf{x}^{(-)}(t_i), \tau = 0) \tag{25}$$

with inverse

$$\mathbf{x}^{(+)}(t_i) \rightarrow \mathbf{x}^{(-)}(t_i) \equiv \chi(\mathbf{x}^{(+)}(t_i), \tau = 0), \tag{26}$$

which are referred to respectively as direct and inverse collision laws.

It is immediate to show that (direct and inverse) collision laws can be uniquely prescribed for all collision events, thus warranting the achievement of *GOAL #1.* To reach the proof, we distinguish for this purpose single and multiple collision events occurring at a given collision time $t_i \in \{t_i\}$. The first type corresponds either to:

- *single binary elastic collision,* in which two hard spheres (particles 1 and 2) mutually collide with each other in such a way to conserve total linear momentum and kinetic energy, namely

$$\sum_{i=1,2} E_i^{(+)} = \sum_{i=1,2} E_i^{(-)}, \tag{27}$$

$$\sum_{i=1,2} \mathbf{v}_i^{(+)} = \sum_{i=1,2} \mathbf{v}_i^{(-)}. \tag{28}$$

Such a collision event is denoted in the following with the symbol $(1-2)$.

- *single unary elastic collision*, in which a single hard sphere (particle 1) collides with the boundary. In this case the conserved dynamical variables are instead respectively

$$E_1^{(+)} = E_1^{(-)}, \tag{29}$$

$$\left|v_{1\|}^{(+)}\right| = \left|v_{1\|}^{(-)}\right| \tag{30}$$

$$\mathbf{v}_{1\perp}^{(+)} = \mathbf{v}_{1\perp}^{(+)}. \tag{31}$$

where $v_{1\|}^{(\pm)} \equiv \mathbf{n}\cdot\mathbf{v}_1^{(\pm)}$ and $\mathbf{v}_{1\perp}^{(\pm)} = \mathbf{v}_1^{(\pm)} - \mathbf{nn}\cdot\mathbf{v}_1^{(\pm)}$(single unary collision).

Let us denote $\mathbf{v}_{12}^{(\pm)} = \mathbf{v}_1^{(\pm)} - \mathbf{v}_2^{(\pm)}$, while $\mathbf{n}_{12} = \mathbf{r}_{12}/\left|\mathbf{r}_{12}\right|$ (with $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$) and $\mathbf{n}$ are the unit vectors, respectively connecting the centers of particles in mutual contact 1 and 2, and orthogonal to the boundary at the position of instantaneous contact of the particle surface $\mathbf{r}_{1w}$.Then, the direct collision laws for single binary or unary collision events are well known (see Ref. [1]). These are given respectively by the equations

$$\begin{cases} \mathbf{r}_1^{(+)} = \mathbf{r}_1^{(-)} = \mathbf{r}_1 \\ \mathbf{r}_2^{(+)} = \mathbf{r}_2^{(-)} = \mathbf{r}_2 = \mathbf{r}_1 + \sigma\mathbf{n}_{21} \\ \mathbf{v}_1^{(+)} = \mathbf{v}_1^{(-)} - \mathbf{n}_{12}\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)} \\ \mathbf{v}_2^{(+)} \ \mathbf{v}_2^{(-)} - \mathbf{n}_{21}\mathbf{n}_{21}\cdot\mathbf{v}_{21}^{(-)} \end{cases} \tag{32}$$

$$\begin{cases} \mathbf{r}_1^{(+)} = \mathbf{r}_1^{(-)} = \mathbf{r}_1 = \mathbf{r}_{1w} + \frac{\sigma}{2}\mathbf{n}. \\ \mathbf{v}_1^{(+)} = \mathbf{v}_1^{(-)} - 2\mathbf{nn}\cdot\mathbf{v}_1^{(-)}. \end{cases} \tag{33}$$

with the corresponding inverse collision laws simply obtained exchanging mutually the symbols $(-)$ and $(+)$ in the previous equations. Then by construction, for consistency with the notation that $\mathbf{v}_{12}^{(-)}$ and $\mathbf{v}_1^{(-)}$ (respectively $\mathbf{v}_{12}^{(+)}$ and $\mathbf{v}_1^{(+)}$) must refer to velocities before (after) collision, it must be $\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)} < 0$ and $\mathbf{n}\cdot\mathbf{v}_1^{(-)} < 0$ (respectively $\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(+)} > 0$ and $\mathbf{n}\cdot\mathbf{v}_1^{(+)} > 0$).

Multiple collisions occurring for the set S_N are regarded as sequences of single collision events, i.e., either unary or binary, occurring simultaneously. It is worth stressing that such sequences, unless they are independent, i.e., involve different sets of particles, must generally be suitably ordered. This means that they generally correspond to a unique and well-defined permutation of particles, with single collision events taking place in a suitable ordered sequence among them. In other words, consistent with the Newton's deterministic principle, even if the set S_N is considered made of like particles, the same particles nevertheless must be regarded as classically distinguishable so that the distinction among all possible collision sequence still obviously holds.

As an illustration, let us consider the example- case of the multiple collision occurring among three particles $(1-2-3)$ in which the simultaneous single binary collisions $(1-2)$ and $(2-3)$ occur (see figure). This means that the two couples of particles $(1,2)$ and $(2,3)$ are in simultaneous mutual contact so that for all $i = 1,3$ there it follows that $\mathbf{r}_i^{(+)} = \mathbf{r}_i^{(-)} = \mathbf{r}_i$, with

$$\begin{aligned} \mathbf{r}_2 &= \mathbf{r}_1 + \sigma\mathbf{n}_{21}, \\ \mathbf{r}_3 &= \mathbf{r}_2 + \sigma\mathbf{n}_{32}, \end{aligned} \tag{34}$$

while the two inequalities

$$\begin{aligned} \mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)} &< 0, \\ \mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)} &< 0, \end{aligned} \tag{35}$$

must both hold too. Indeed, thanks to (35), both $\mathbf{v}_{12}^{(-)}$ and $\mathbf{v}_{23}^{(-)}$ can then to be regarded as the relative velocities of the incoming particles (i.e., before the occurrence of the multiple collision event). In principle, such an event can be either realized by the means of ordered sequences of single binary collisions, namely either $[(1-2),(2-3)]$ or instead $[(2-3),(1-2)]$, in which respectively the single binary collision $(1-2)$ is considered as occurring respectively before or after $(2-3)$. In terms of Eq. (32 in the first case the corresponding direct collision laws are provided, together

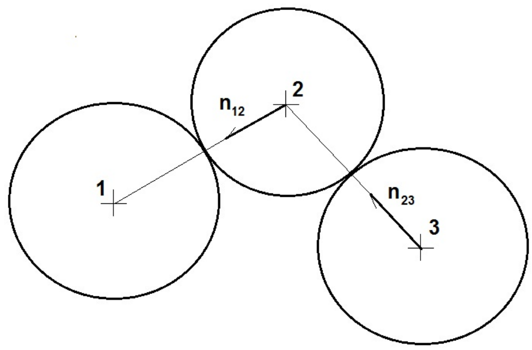

FIG. 1: Case of double binary collision

with Eqs. (34), by the velocity transformation laws

$$\begin{aligned}
\mathbf{v}_1^{(+)} &= \mathbf{v}_1^{(-)} - \mathbf{n}_{12}\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)}, \\
\mathbf{v}_2^{(+)} &= \mathbf{v}_2^{(-)} - \mathbf{n}_{21}\mathbf{n}_{21}\cdot\mathbf{v}_{21}^{(-)} - \mathbf{n}_{23}\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)} + \mathbf{n}_{32}\mathbf{n}_{12}\cdot\mathbf{n}_{32}\mathbf{n}_{32}\cdot\mathbf{v}_{32}^{(-)}, \\
\mathbf{v}_3^{(+)} &= \mathbf{v}_3^{(-)} - \mathbf{n}_{32}\mathbf{n}_{32}\cdot\mathbf{v}_{32}^{(-)} - \mathbf{n}_{32}\mathbf{n}_{12}\cdot\mathbf{n}_{32}\mathbf{n}_{32}\cdot\mathbf{v}_{32}^{(-)},
\end{aligned} \tag{36}$$

which require also the validity of the subsidiary condition

$$\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)} - \mathbf{n}_{12}\cdot\mathbf{n}_{32}\mathbf{n}_{32}\cdot\mathbf{v}_{32}^{(-)} < 0. \tag{37}$$

Instead, in the second case the velocity transformation laws become

$$\begin{aligned}
\mathbf{v}_1^{(+)} &= \mathbf{v}_1^{(-)} - \mathbf{n}_{12}\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)} - \mathbf{n}_{12}\mathbf{n}_{12}\cdot\mathbf{n}_{23}\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)}, \\
\mathbf{v}_2^{(+)} &= \mathbf{v}_2^{(-)} - \mathbf{n}_{21}\mathbf{n}_{21}\cdot\mathbf{v}_{21}^{(-)} - \mathbf{n}_{23}\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)} + \mathbf{n}_{21}\mathbf{n}_{21}\cdot\mathbf{n}_{23}\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)}, \\
\mathbf{v}_3^{(+)} &= \mathbf{v}_3^{(-)} - \mathbf{n}_{32}\mathbf{n}_{32}\cdot\mathbf{v}_{32}^{(-)},
\end{aligned} \tag{38}$$

along with the corresponding subsidiary condition

$$\mathbf{n}_{12}\cdot\mathbf{v}_{12}^{(-)} - \mathbf{n}_{12}\cdot\mathbf{n}_{23}\mathbf{n}_{23}\cdot\mathbf{v}_{23}^{(-)} < 0. \tag{39}$$

The previous equations (34), together with either (36) or (38), provide possible realizations of the direct collision law for the multiple collision. The corresponding inverse collision laws follow also in this case by simply exchanging the symbols $(-)$ and $(+)$ in the previous equations.

Analogous conclusions can be inferred also in the case of arbitrary multiple collisions. Hence collision laws corresponding to different sequences of single collisions lead generally to different outgoing velocities of colliding particles. As a consequence we conclude that:

1) to prescribe uniquely the time evolution of the S_N-CDS the distinction between all possible ordered sequences of single (unary and binary) collisions must be made. Such a choice is manifestly consistent with the validity of Newton's deterministic principle for classical dynamical systems.

2) the validity itself of the statistical principle of classical indistinguishability [31] might seem to be put in question at this stage (see discussion below in Sec. 6).

4 - GLOBAL UNIQUE PRESCRIPTION OF THE GENERIC $N-$BODY PDF

The problem to be posed in the present section and in the following one concerns the determination of particular realizations of the $N-$body PDF which are globally defined. Here we shall deal, in particular, with generic (i.e., arbitrary) realizations of the solution of the Γ_N-phase-space Liouville equation for the S_N-CDS which belong to the extended functional setting indicated above (*GOAL #2*). The latter equation, written in Eulerian form and holding in the collisionless subset $\overline{\Gamma}_N$ (see definition in the Appendix), reads

$$L_N \rho^{(N)}(\mathbf{x}, t) = 0, \tag{40}$$

where $L_N = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}}$ is the $N-$body free-streaming operator, with $\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \equiv \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i}$ and the summation on repeated indices is understood. Regarding the problem of global existence for such an equation, one has to recognize that the first attempt of this type to be found in the literature is that due to Harold Grad with his paper on the *Principles of Kinetic Theory* [25]. His approach, which subsequently has been very influential to both the physical and mathematical communities, was based in fact on the same Liouville equation. It is interesting to point out, however, that in his approach actually Grad adopted the same type of functional setting based on the PDF-conserving collision boundary condition recalled above (see Eq. (3)), originally introduced by Boltzmann [7] for the statistical treatment of particle collisions. The same route was followed also in the subsequent literature (see for example Cercignani [17]). Actually, as shown in Ref. [4], one can readily reconstruct the key assumption, underlying Grad's approach, which led him to such a choice for the CBC. This requires, first, to represent the $N-$body PDF and the same Liouville equation (40) in Lagrangian form, i.e., both parametrized in terms of the phase-space Lagrangian trajectory $\mathbf{x}(t)$, with $\mathbf{x}(t)$ in turn being uniquely prescribed by the S_N-CDS. Thus, one obtains $\rho^{(N)} = \rho^{(N)}(\mathbf{x}(t), t)$ and

$$\frac{d}{dt} \rho^{(N)}(\mathbf{x}(t), t) = 0, \tag{41}$$

respectively, the latter identifying the Lagrangian differential Liouville equation. Notice that manifestly Eq. (41) holds only in all collisionless open time intervals $\widehat{I}_i =]t_i, t_{i+1}[$, with arbitrary $i \in \mathbb{Z}$, defined between two successive collision times $t_i, t_{i+1} \in I$. Eq. (41) can formally be integrated in each collisionless time interval $\widehat{I}_i$, to give for all $t, t+\tau \in \widehat{I}_i$

$$\rho^{(N)}(\mathbf{x}(t), t) = \rho^{(N)}(\mathbf{x}(t+\tau), t+\tau), \tag{42}$$

with $\mathbf{x}(t)$ and $\mathbf{x}(t+\tau)$ being the corresponding states of the S_N-CDS. Therefore, to obtain the global time evolution of the Lagrangian PDF $\rho^{(N)}(\mathbf{x}(t), t)$ it is mandatory to prescribe also the appropriate CBC. In Grad's original approach the *global unique prescription* of $\rho^{(N)}(\mathbf{x}(t), t)$ was actually achieved by requiring the same PDF to satisfy the integral Liouville equation (42) in a "global sense", i.e., requiring also that at all collision times $t_i \in \{t_i\}$ the PDF-conserving CBC Eq. (3) is fulfilled. Nevertheless, although Eq. (3) can be viewed as a restatement of the Liouville equation valid across collision times, its fulfillment is actually not required for the validity of the statistical treatment of the S_N-CDS [2, 4]. Instead, on the contrary, Eq. (3) is in conflict with the basic physical requirement that the deterministic $N-$body PDF be a particular solution of the Liouville equation.

The solution of the issue can be reached adopting the new "*ab initio*" approach to CSM [1–6], based in particular on the introduction of the modified CBC represented by Eq. (6). If the property of left continuity at all collision times $\rho^{(-)(N)}(\mathbf{x}^{(-)}(t_i), t_i)$ is invoked for $\rho^{(-)(N)}$ the previous left limit can be replaced with $\rho^{(N)}(\mathbf{x}^{(-)}(t_i), t_i)$ so that Eq. (6) yields:

$$\rho^{(+)(N)}(\mathbf{x}^{(+)}(t_i), t_i) = \rho^{(N)}(\mathbf{x}^{(+)}(t_i), t_i). \tag{43}$$

By construction such a CBC has the following features:

- it applies *at arbitrary collision times* $t_i \in \{t_i\}$ and hence correspondingly for *arbitrary collision events.*
- it is *unique.*
- it realizes the *causal form* of MCBC, which advances in time the outgoing PDF in terms of the incoming one.
- it holds, unlike Eq. (3), for distributions such as the deterministic $N-$body PDF.
- as shown in Ref. [2] for a generic PDF, i.e., an *arbitrary realization of the N-body PDF* which belongs to the *extended functional setting* here adopted, it realizes - in a strict sense - the only *physically-admissible* CBC.

It must be stressed that, as discussed in Refs. [3] and [6], in validity of the dilute-gas asymptotic approximation the distinction between MCBC and PDF-conserving CBC may become effectively irrelevant from the physical standpoint. This happens because in the case of suitably smooth stochastic PDFs the finite-size of hard sphere does not matter any more in the statistical description of hard-sphere collisions (see related discussions in Refs. [1, 3, 6]. Nevertheless, from the mathematical viewpoint the distinction between the two types of CBC remains crucial. In fact, it is only MCBC which warrants the unique time-advancement of the $N-$body PDF at all collision times.

The fundamental implication is therefore that in the framework of the extended functional setting here introduced global existence of solutions for the Liouville equation is warranted *only if* MCBC is invoked (*GOAL #2*). As a result, the generic $N-$body PDF by construction can belong in principle both to the class of ordinary functions, being identified with a stochastic PDFs, as well as distributions, such as the deterministic and partially deterministic $N-$body PDFs.

5 - GLOBAL UNIQUE PRESCRIPTION OF FACTORIZED EXTREMAL $N-$BODY PDFS

Let us now analyze in detail a novel feature of the axiomatic "ab initio" statistical description developed in Ref. [1] with respect to the customary treatment (see Ref. [25]). As recalled by *Result #3,* this lies in the existence of exact permutation-symmetric solutions of the Γ_N-phase-space Liouville equation for the S_N-CDS which are factorized in terms of the $1-$body PDFs associated with the ensemble of like particles S_N. Such particular solutions can be realized in principle either by stochastic, deterministic or partially determinist $N-$body PDFs. In the first case, provided the initial $1-$ and $N-$ body PDFs both admit the corresponding $1-$ and $N-$body Boltzmann-Shannon entropies, one can show that the same $N-$ body PDF is also extremal since it satisfies at the initial time $t=t_o$ the so-called maximal principle of entropy maximization (PEM; [3]). Remarkably, as a consequence of the entropic theorems discovered in Ref. [6], this means that the corresponding time-advanced $N-$ body PDF remains maximal in the same sense at any time t which belongs to its domain of existence In this section we intend to show that such a domain coincides with the time axis $I\equiv\mathbb{R}$, global existence being again consequence of the global prescription of the S_N-CDS as well as the validity of MCBC (*GOAL #3*).

Indeed, one preliminarily must notice that example of factorized particular solution arises naturally in the case of the deterministic $N-$body PDF $\rho_H^{(N)}$, which by construction is the product of the corresponding $1-$particle deterministic PDFs $\rho_{H1}^{(N)}(\mathbf{x}_i,t)$ for all $i=1,N$ (see Eq. (5)). In the phase-space Γ_N this can be equivalently represented as

$$\rho_H^{(N)}(\mathbf{x},t)=\overline{\Theta}^{(N)}(\mathbf{r},t)\prod_{i=1,N}\rho_{H1}^{(N)}(\mathbf{x}_i,t). \tag{44}$$

It is therefore natural to conjecture the existence of a stochastic PDF which is of the type

$$\rho^{(N)}(\mathbf{x},t)=\overline{\Theta}^{(N)}(\mathbf{r},t)\widehat{\rho}^{(N)}(\mathbf{x},t), \tag{45}$$

with $\widehat{\rho}^{(N)}(\mathbf{x},t)$ being a factorized solution of the form

$$\widehat{\rho}^{(N)}(\mathbf{x},t)=\prod_{i=1,N}\frac{\rho_1^{(N)}(\mathbf{x}_i,t)}{k_1^{(N)}(\mathbf{r}_i,t)} \tag{46}$$

and $\rho_1^{(N)}(\mathbf{x}_1,t)$ the $1-$body PDF. The requirement that

$$\rho_1^{(N)}(\mathbf{x}_1,t)=F_1\left\{\rho^{(N)}(\mathbf{x},t)\right\} \tag{47}$$

implies necessarily that Eq. (14) for $k_1^{(N)}(\mathbf{r}_1,t)$ is necessarily fulfilled too, $k_1^{(N)}(\mathbf{r}_1,t)$ identifying the $1-$ *body occupation coefficient [3],* physically related to the occupation domain of the hard spheres arising due to their finite size. This means that the same coefficient is uniquely determined by the integral equation (14), **namely**

$$k_1^{(N)}(\mathbf{r}_1,t)=\int\limits_{\Gamma_{1(2)}}d\mathbf{x}_2\frac{\rho_1^{(N)}(\mathbf{x}_2,t)}{k_1^{(N)}(\mathbf{r}_2,t)}\overline{\Theta}_2\left(\mathbf{r}_1,\mathbf{r}_2\right)...\int\limits_{\Gamma_{1(N)}}d\mathbf{x}_N\frac{\rho_1^{(N)}(\mathbf{x}_N,t)}{k_1^{(N)}(\mathbf{r}_N,t)}\overline{\Theta}_N\left(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_N\right). \tag{48}$$

It must also be noticed that the factorization conditions (10) and (46) prescribe the $N-$body PDF in terms of the $1-$body PDF $\rho_1^{(N)}(\mathbf{x}_i,t)$ and the occupation coefficients $k_1^{(N)}$ respectively at the initial time t_o and at a generic time t. On the other hand, the precise form of the $1-$body PDF $\rho_1^{(N)}(\mathbf{x}_i,t)$ remains arbitrary in the present treatment. As a result, the theory developed here does not preclude the possibility of having both Maxwellian as well as non-Maxwellian $1-$body stochastic distribution functions as well as distributions. This feature is particularly relevant for the treatment of granular flows, where the occurrence of non-Maxwellian velocity distributions is naturally observed [35–39].

It is possible to prove that the factorized solution (45) satisfies the fundamental axiom of probability conservation and in addition is consistent with MCBC. The proof is given by THM.2 and 3 reported in Ref. [3]. The implications are as follows. Let us assume, for definiteness, that the initial conditions of $\rho^{(N)}(x,t)$ are prescribed according to (10). Then, noting that by construction one can always requite the condition of left-continuity $\widehat{\rho}^{(-)(N)}(\mathbf{x}^{(-)}(t_i),t_i) = \widehat{\rho}^{(N)}(\mathbf{x}^{(-)}(t_i),t_i)$, the *Lagrangian PDF* $\rho^{(N)}(\mathbf{x}(t),t)$ *is uniquely and globally prescribed so that its domain of existence coincides with* $I\equiv\mathbb{R}$ *(GOAL #3)*. Indeed:

1) At arbitrary collision times $t_i\in\{t_i\}$ and hence correspondingly for arbitrary collision events the outgoing PDF $\widehat{\rho}^{(+)(N)}(\mathbf{x}^{(+)}(t),t)$ is determined by the causal Lagrangian form of MCBC, yielding

$$\widehat{\rho}^{(+)(N)}(\mathbf{x}^{(+)}(t_i),t_i) = \widehat{\rho}^{(N)}(\mathbf{x}^{(+)}(t_i),t_i) \tag{49}$$

and hence the outgoing PDF remains uniquely factorized.

2) At an arbitrary $t\neq t_o$, with $t\in I-\{t_i\}$, the $N-$body PDF is factorized too with respect to the state $\mathbf{x}(t)$, image of $\mathbf{x}_o$ determined again by the S_N-CDS, so that in Lagrangian form it reads .

$$\rho^{(N)}(\mathbf{x}(t),t) = \overline{\Theta}^{(N)}(\mathbf{r}(t),t)\widehat{\rho}^{(N)}(\mathbf{x}(t),t), \tag{50}$$

with $\widehat{\rho}^{(N)}(\mathbf{x},t)$ given by Eq.(46).

The previous statements manifestly hold for arbitrary phase-space trajectories $\mathbf{x}(t)$ of the S_N-CDS so that in arbitrary collisioness time intervals $\widehat{I}_i\subset I$ the factorized extremal solution (45)-(46) identically satisfies also the differential Liouville equation in Lagrangian form, namely:

$$\frac{d}{dt}\widehat{\rho}^{(N)}(\mathbf{x}(t),t) = 0. \tag{51}$$

6 - GLOBAL UNIQUE EXISTENCE PROBLEM FOR THE MASTER KINETIC EQUATION

In this section we investigate the consequences of the global existence of factorized $N-$body PDF particular solutions of the Γ_N-phase-space Liouville equation which are of the type (45)-(46). First we notice that, thanks to the Lagrangian Liouville equation (51), it follows that the same equation must of course hold also in Eulerian form. This implies therefore that in the collisionless subset $\overline{\Gamma}_N$ the $N-$particle PDF given by Eqs. (45)-(46) necessarily satisfies the Eulerian Liouville equation

$$L_N\widehat{\rho}^{(N)}(\mathbf{x},t) = 0, \tag{52}$$

which is therefore identically, i.e., globally in time, satisfied. As shown in Ref. [3] it is immediate to prove that the same equation (52) implies also that the corresponding $1-$body PDF$\rho_1^{(N)}(\mathbf{x}_i,t)$ must satisfy a well-defined differential equation, referred to as the Master kinetic equation. The result is established by THM.5 in Ref. [37]. Indeed Eq. (52) requires

$$\frac{d}{dt}\widehat{\rho}^{(N)}(\mathbf{x}(t),t) = \sum_{i=1,N} L_{1(i)}\left\{\frac{\rho_1^{(N)}(\mathbf{x}_i,t)}{k_1^{(N)}(\mathbf{r}_i,t)}\right\}\prod_{j=1,N,j\neq i}\frac{\rho_1^{(N)}(\mathbf{x}_j,t)}{k_1^{(N)}(\mathbf{r}_j,t)} = 0 \tag{53}$$

to hold, which requires that for all $i=1,N$, $\rho_1^{(N)}(\mathbf{x}_i,t)$ must fulfill the exact kinetic equation

$$L_{1(i)}\frac{\rho_1^{(N)}(\mathbf{x}_i,t)}{k_1^{(N)}(\mathbf{r}_i,t)} = 0, \tag{54}$$

referred to as the first form Master kinetic equation. According to Refs. [3, 4], Eq.(54) is equivalently realized by the evolution equation , namely

$$L_1\rho_1^{(N)}(\mathbf{x}_1,t)=\mathcal{C}_1\left(\widehat{\rho}_1^{(N)}|\widehat{\rho}_1^{(N)}\right). \tag{55}$$

which identifies the so-called second form of the Master kinetic equation first introduced in Ref. [3]. Here $L_1\equiv\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\frac{\partial}{\partial\mathbf{r}_1}$ and $\mathcal{C}_1\left(\widehat{\rho}_1^{(N)}|\widehat{\rho}_1^{(N)}\right)$ denote respectively the 1−body free-streaming operator and

$$\mathcal{C}_1\left(\widehat{\rho}_1^{(N)}|\widehat{\rho}_1^{(N)}\right)=\int\limits_{\Gamma_{1(2)}}^{(-)}d\mathbf{x}_2\delta\left(|\mathbf{r}_2-\mathbf{r}_1|-\sigma\right)\overline{\Theta}\left(\left|\mathbf{r}_2-\frac{\sigma}{2}\mathbf{n}_2\right|-\frac{\sigma}{2}\right)T_{12}(\mathbf{x}_1,\mathbf{x}_2,t), \tag{56}$$

with $T_{12}(\mathbf{x}_1,\mathbf{x}_2,t)$ being the integrand

$$\begin{gathered}T_{12}(\mathbf{x}_1,\mathbf{x}_2,t)\equiv(N-1)\left|\mathbf{v}_{21}\cdot\mathbf{n}_{21}\right| \\ \left[\widehat{\rho}_1^{(N)}(\mathbf{x}_1^{(+)},t)\widehat{\rho}_1^{(N)}(\mathbf{x}_2^{(+)},t)-\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t)\widehat{\rho}_1^{(N)}(\mathbf{x}_2,t))\right]\frac{k_2^{(N)}(\mathbf{r}_1,\mathbf{r}_2,t)}{k_1^{(N)}(\mathbf{r}_1,t)k_1^{(N)}(\mathbf{r}_2,t)},\end{gathered} \tag{57}$$

while $k_1^{(N)}(\mathbf{r}_1,t)$ and $k_2^{(N)}(\mathbf{r}_1,\mathbf{r}_2,t)$ are given by Eqs. (14) and (15). Regarding, in particular, the mathematical properties of Eq. (55), it should be recalled that, being a particular solution of the $N-$body Liouville equation, $\rho^{(N)}(\mathbf{x},t)$ is by construction unique and globally defined, i.e., it exists for all t belonging to the time axis $I\equiv\mathbb{R}$. In fact, as shown in Ref. [3], while all Lagrangian trajectories associated with the S_N-CDS are by assumption unique, along the same trajectories $\rho^{(N)}(\mathbf{x},t)$ remains by construction constant in the absence of collisions, while - thanks to the requirement posed by the validity of MCBC - its functional form is preserved during arbitrary collision events. On the other hand, Eqs. (49) and (50) manifestly imply that both $\rho_2^{(N)}(\mathbf{x}_1,\mathbf{x}_2,t)$ and $\rho_1^{(N)}(\mathbf{x}_1,t)$ remain necessarily uniquely globally-defined. Hence, by construction the solution $\rho_1^{(N)}(\mathbf{x}_1,t)$ of Eq. (55) is manifestly unique and holds globally in time too. Furthermore, as shown in Refs. [3, 4], $\rho^{(N)}(\mathbf{x},t)$ admits both stochastic as well as deterministic possible particular realizations. The latter is given by the so-called deterministic $N-$body PDF (or certainty function according to Ref. [20]) given in Refs. [1, 3].

Then, the following proposition holds.

THM.1 - Global validity of the Master kinetic equation and Master H-theorem

Eq.(55) realizes a hyperbolic evolution equation for the $1-$*body (kinetic) PDF* $\rho_1^{(N)}(\mathbf{x}_1,t)$ *which corresponds to an* $N-$*body PDF of the form (45)-(46) , i.e., an equation whose solution* $\rho_1^{(N)}(\mathbf{x}_1,t)$ *is by construction unique and globally-defined. In particular, if the initial* $N-$*body PDF* $\rho_1^{(N)}(\mathbf{x},t_o)$ *is assumed to be a stochastic PDF which is strictly positive and summable in the admissible subset of the phase-space* Γ_N *in the sense that it admits and maximizes all corresponding* $s-$*body Boltzmann-Shannon entropies which for all* $s=1,N$ *are associated with the* $s-$*body PDF* $\rho_s^{(N)}(\mathbf{x}_1,...,\mathbf{x}_s,t_o)$*, then it follows necessarily that:*

$P1_1$) ***Master kinetic equation:*** *both* $\rho^{(N)}(\mathbf{x},t)$ *and the corresponding* $1-$*body PDF* $\rho_1^{(N)}(\mathbf{x}_1,t)$ *realize, in the whole extended phase spaces* $\Gamma_N\times I$ *and* $\Gamma_{1(1)}\times I$ *respectively, uniquely-related stochastic and globally strictly positive PDFs.*

$P1_2$) ***Master H-theorem:*** *the* $s-$*body Boltzmann-Shannon entropies associated with* $\rho_s^{(N)}(\mathbf{x}_1,...,\mathbf{x}_s,t)$*, are defined and constant for all* $s=1$ *and for all* $t\in I$*,*

Proof - Following the guidelines pointed out in Ref. [3] the proof-strategy of the global validity for the solution of the Master kinetic equation (i.e., proposition $P1_1$) is conceptually straightforward. The goal, in fact, is reached by inspecting the $N-$body Liouville equation for the factorized solution (45)-(46), where for definiteness the initial $N-$body PDF $\rho^{(N)}(\mathbf{x},t_o)$ can be assumed to be summable in the admissible subset of the $N-$body phase-space Γ_N in the sense that it admits for all $s=1,N$ also the $s-$body BS entropy integrals (see Ref. [6]) . As discussed in the same reference, the $N-$body Liouville equation can be equivalently represented in integral (or differential) Lagrangian and differential Eulerian forms. According to the integral Lagrangian representation, during an arbitrary open collisionless time interval, occurring between two consecutive collision times $\widehat{I}_i\equiv]t_i,t_{i+1}[$, for all $t,t+\tau\in\widehat{I}_i$ it must occur that $\rho^{(N)}(\mathbf{x}(t),t)$ remains constant, i.e.,

$$\rho^{(N)}(\mathbf{x}(t),t)=\rho^{(N)}(\mathbf{x}(t+\tau),t). \tag{58}$$

Instead at arbitrary collision times the causal form of the collision boundary condition, which determines the (outgoing) PDF $\rho^{(+)(N)}$ after collision in terms of the corresponding (incoming) one $\rho^{(-)(N)} \equiv \rho^{(N)}$ before collision**,** is provided by MCBC [1, 2]. In Lagrangian form it is realized by the equation Eq. (6). As pointed out in the previous section the time-evolution of the factorized $N-$body PDF is globally uniquely determined, once the initial factorized PDF $\rho^{(N)}(\mathbf{x},t_o)$ is suitably prescribed in accordance with Eqs. (10). Hence, along arbitrary Lagrangian trajectories $\{\mathbf{x}(t)\}$ of the S_N-CDS, $\rho^{(N)}(\mathbf{x}(t),t)$ remains uniquely globally prescribed. This implies that in the whole admissible subset of the phase-space Γ_N the $N-$body PDF is everywhere of the form (45)-(46), and hence in particular it is stochastic, strictly positive and summable in the sense indicated above. On the other hand as shown again in Ref. [3], when cast in Eulerian form and represented in terms of the same factorized solution, the $N-$body Liouville equation is equivalent to the Master kinetic equation (55). The proof of proposition $P1_2$), i.e., the global validity of the Master H-theorem follows instead noting that the entropy production rate identically vanishes, i.e.,

$$\frac{\partial}{\partial t}S_s(\widehat{\rho}_s^{(N)}(t))=0, \tag{59}$$

where $\widehat{\rho}_s^{(N)}(t)(\equiv\rho_s^{(N)}(\mathbf{x}^{(s)},t))\equiv F_s\left\{\widehat{\rho}^{(N)}(t)\right\}$ is prescribed in terms of the factorized $N-$body PDF Eqs. (45)-(46) (see related proof given by THM.3 in Ref. [6]). Q.E.D.

Before concluding this section a few comments are appropriate.

The first one is the remark that THM.1, i.e., the validity of an Eulerian kinetic equation to be identified with the Master kinetic equation, is an obvious consequence of the global existence of factorized solutions of type (45)-(46) for the $N-$body PDF. In particular, both in the Lagrangian and Eulerian descriptions the explicit time-dependences occurring in the $N-$ and $1-$body PDF are produced by collisions.

The second comment is that the second form of the Master equation (see Eq. (55)) can be reached, as shown in Ref. [3], in two equivalent ways: 1) The first one is obtained by applying the integral operator F_1 to the Liouville Eq. (52) , i.e., constructing the corresponding equation of the BBGKY hierarchy and in the process taking into account also MCBC (see Refs. [3, 4]). 2) The second approach, yielding the same conclusion, follows also by making use of the first form of the Master kinetic equation (see Eq. (54)), i.e., again, once MCBC is consistently dealt with.. Consider, for example, the first route. For this purpose, in view of Eqs. (14) and (48), one needs to evaluate explicitly the action of the differential operator $L_{1(i)}$ on the occupation coefficient $k_1^{(N)}(\mathbf{r}_i,t)$, namely

$$L_{1(1)}k_1^{(N)}(\mathbf{r}_1,t)=L_{1(1)}F_1\left\{\prod_{j=2,N}\frac{\rho_1^{(N)}(\mathbf{x}_j,t)}{k_1^{(N)}(\mathbf{r}_j,t)}\right\}. \tag{60}$$

The third comment concerns the issue related to the validity of the principle of classical indistinguishability [31] mentioned at the end of Section 3. The answer to this question lies in the observation that actually in case of stochastic $1-$body PDF only single binary collisions affect the Eulerian time-dependence appearing in the same PDF. This feature is manifest by direct inspection of the Master collision operator (see Eq.(56)). The same conclusion can be shown to be consistent with the analogous property of the equations of the differential BBGKY hierarchy. For the same BBGKY hierarchy such a feature, first discovered by Grad [25], turns out to be actually independent of the type of the adopted CBC (see in this regard the extended related discussion reported in Ref. [4]). Finally, the fourth comment is related to the implications of the Master H-theorem. As discussed in Refs. [5, 6] one can show, in fact, the global validity of the maximal form of PEM recalled above (see Result #1). In other words, thanks to the Master H-theorem, such a principle holds in principle at any initial time $t_o\in I$, i.e., of course provided the initial $1-$body PDF at time t_o is suitably prescribed too.

7 - IMPLICATIONS FOR THE ASYMPTOTIC BOLTZMANN KINETIC EQUATION AND BOLTZMANN H-THEOREM

In this section the asymptotic approximation scheme appropriate for describing the dilute-gas asymptotic ordering (see Introduction) is recalled [6]. In fact. as pointed out in the introduction (see issue #4), from the physical standpoint the notion of Boltzmann-Grad limit must necessarily be replaced by an asymptotic ordering condition of the type (17). In contrast to the Boltzmann-Grad limit, this means that both $\varepsilon\equiv\frac{1}{N}$ and the molecular diameter σ are to be regarded as finite, despite being ordered in the asymptotic sense prescribed by Eqs. (17). In principle a number of important questions may arise regarding the dilute-gas asymptotic kinetic theory. Here, we intend to investigate, in particular, the implications for the asymptotic Boltzmann equation and the corresponding asymptotic Boltzmann

H-theorem which as shown in Ref. [6] can be obtained under suitable conditions from the Master equation and the Master H-theorem respectively.

To address the issue we introduce the following set of asymptotic approximations which are assumed to apply in validity of the dilute-gas ordering (17). Consistent with the assumptions introduced in Ref. [3], these concern in detail:

1) *Smoothness conditions holding for the* $1-$ and $2-$*body occupation coefficients* $k_1^{(N)}(\mathbf{r}_1,t)$ and $k_2^{(N)}(\mathbf{r}_1,\mathbf{r}_2,t)$. We require the asymptotic estimates

$$\begin{gathered} k_1^{(N)}(\mathbf{r}_1,t)=1+O(\varepsilon^{1/2}), \\ k_2^{(N)}(\mathbf{r}_1,\mathbf{r}_2,t)=1+O(\varepsilon^{1/2}), \end{gathered} \tag{61}$$

to hold.

2) *Smoothness conditions for the* $1-$body PDF $\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t)\equiv\widehat{\rho}_1^{(N)}(\mathbf{r}_1,\mathbf{v}_1,t)$, namely respectively

$$\rho_1^{(N)}(\mathbf{r}_2=\mathbf{r}_1+\sigma\mathbf{n}_{21},\mathbf{v}_2^{(+)},t)=\rho_1^{(N)}(\mathbf{r}_2=\mathbf{r}_1,\mathbf{v}_2^{(+)},t))\left[1+O\left(\varepsilon^{1/2}\right)\right]. \tag{62}$$

Here $\rho_1(\mathbf{x}_1,t)$ denotes a particular solution of the asymptotic Boltzmann kinetic equation (see below), whose initial condition is set prescribing $\rho_1(\mathbf{x}_1,t_o)\equiv\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t_o)$, with $\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t_o)$ denoting the initial $1-$body PDF.

3) *Regularity condition requiring the negligible contribution of the excluded sub-domains associated with* $\overline{\Theta}_{2(1)}(\mathbf{r})$, whereby in the Master collision operator the contribution

$$\overline{\Theta}\left(\left|\mathbf{r}_2-\frac{\sigma}{2}\mathbf{n}_2\right|-\frac{\sigma}{2}\right)=1+O(\varepsilon^{1/2}), \tag{63}$$

can be regarded as being effectively replaced with $\overline{\Theta}_{2(1)}(\mathbf{r})=1$. As shown in Ref. [6], it is immediate to **prove** that in validity of the asymptotic approximations 1-3, $\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t)$ is an asymptotic solution of the Boltzmann equation and that analogously it satisfies in an asymptotic sense also the Boltzmann H-theorem. Indeed, if $\rho_1^{(N)}(\mathbf{x}_1,t)$ is a particular stochastic PDF solutions of the Master equation (whose global existence is warranted by THM.1) the asymptotic relationship

$$\rho_1^{(N)}(\mathbf{r}_1,\mathbf{v}_1,t)=\rho_1(\mathbf{r}_1,\mathbf{v}_1,t)\left[1+O\left(\varepsilon^{1/2}\right)\right] \tag{64}$$

holds, with ρ_1 denoting a particular solution of the *asymptotic Boltzmann kinetic equation*, namely

$$L_1\rho_1(\mathbf{x}_1,t)=\mathcal{C}_B\left(\rho_1|\rho_1\right)\left[1+O\left(\varepsilon^{1/2}\right)\right]. \tag{65}$$

Notice that in particular $\rho_1(\mathbf{r}_1,\mathbf{v}_1,t)$ can also be required to satisfy the same initial conditions

$$\rho_1(\mathbf{x}_1,t_o)=\rho_{1(o)}^{(N)}(\mathbf{x}_1)=\rho_1^{(N)}(\mathbf{x}_1,t_o), \tag{66}$$

by assumption are obeyed by $\rho_{11}^{(N)}(\mathbf{x}_1,t)$. The global existence problems for the asymptotic equation (65) is of course meaningful only provided the set of asymptotic approximations indicated above (see Eqs. (61)-(63)) actually globally applies. In such a case the following proposition holds.

THM.2 - Global validity of the asymptotic Boltzmann equation and Boltzmann H-theorem

In validity of THM.1, let us assume that

1) the dilute-gas asymptotic ordering (17) holds;

2) the approximations (61)-(63) hold identically in the set $\Gamma_{1(1)}\times I$.

Then the following propositions hold globally in the set $\Gamma_{1(1)}\times I$*:*

P2$_1$*) the* $1-$*body PDF* $\rho_1^{(N)}(\mathbf{x}_1,t)\equiv\widehat{\rho}_1^{(N)}(\mathbf{x}_1,t)$ *is an asymptotic solution of the Boltzmann equation, namely it satisfies the asymptotic equation*

$$L_1\rho_1^{(N)}(\mathbf{x}_1,t)=\mathcal{C}_B\left(\rho_1^{(N)}|\rho_1^{(N)}\right)\left[1+O(\varepsilon^{1/2})\right]. \tag{67}$$

P2$_2$*) It follows identically in* $\Gamma_{1(1)}\times I$ *that*

$$\rho_1^{(N)}(\mathbf{x}_1,t)=\rho_1(\mathbf{x}_1,t)\left[1+O(\varepsilon^{1/2})\right], \tag{68}$$

with $\rho_1(x_1,t)$ particular solution of the asymptotic Boltzmann equation (65) which fulfills the initial conditions (66). Hence $\rho_1(\mathbf{x}_1,t)$ identifies a global solution of the asymptotic Boltzmann equation.

$P2_3$) the asymptotic Boltzmann H-theorem

$$\frac{\partial}{\partial t}S_1(\rho_1((t)))\left[1+O(\varepsilon^{1/2})\right]\geq 0 \tag{69}$$

holds globally in time.

Proof - First we notice that the proof of proposition $P2_1$) is an immediate consequence of hypotheses 1) and 2). In fact, in validity of the asymptotic ordering (17) and the asymptotic approximations (61)-(63), one obtains that

$$\mathcal{C}_1\left(\rho_1^{(N)}|\rho_1^{(N)}\right)=\mathcal{C}_B\left(\rho_1^{(N)}|\rho_1^{(N)}\right)\left[1+O(\varepsilon^{1/2})\right], \tag{70}$$

so that Eq. (67), up to contributions of $O(\varepsilon^{1/2})$ identifies indeed the asymptotic Boltzmann equation. As a consequence, the asymptotic approximation (68) manifestly holds ($P2_2$). Notice that here by construction the initial conditions (66) manifestly holds. Finally, the validity of the entropy-rate inequality (69) (Proposition $P2_3$) is immediate (see Ref. [6]). In fact, thanks to the Brillouin Lemma the inequality

$$S_1(\rho_1^{(N)}(t))\leq -\int\limits_{\Gamma_1}d\mathbf{x}_1\rho_1^{(N)}(\mathbf{x}_1,t)\ln\rho_1(\mathbf{x}_1,t) \tag{71}$$

necessarily holds (notice that by construction $\int\limits_{\Gamma_1}d\mathbf{x}_1\rho_1^{(N)}(\mathbf{x}_1,t)=1$). Notice that thanks to the approximation (62)

$$-\int\limits_{\Gamma_1}d\mathbf{x}_1\rho_1^{(N)}(\mathbf{x}_1,t)\ln\rho_1(\mathbf{x}_1,t)=S_1(\rho_1(t))\left[1+O(\varepsilon^{1/2})\right], \tag{72}$$

it follows also that for all $t\in I$

$$S_1(\rho_1^{(N)}(t))\leq S_1(\rho_1(t))\left[1+O(\varepsilon^{1/2})\right], \tag{73}$$

which warrants the validity of proposition $P2_3$ (i.e., of the asymptotic Boltzmann H-theorem (69)). **Q.E.D.**

The following remarks are worth to be mentioned regarding THM.2 and the establishment of the related *GOAL #5.*

Let us first consider Proposition $P2_2$. One notices that being $\rho_1(\mathbf{x}_1,t)$ a solution of the (asymptotic) Boltzmann equation, it actually coincides by construction with the so-called Boltzmann-Grad limit of $\rho_1^{(N)}(\mathbf{x}_1,t)$.As recalled above, in validity of the dilute-gas ordering (17) and asymptotic approximations 1-3, this is obtained by taking the continuum limit $N\rightarrow\infty$. Hence global existence is warranted in principle also in this limit. Analogous conclusions concern the validity of the asymptotic H-theorem (69) in the same limit (Proposition $P2_3$).

The second remark refers to a remaining possibly-fundamental issue. This concerns the actual proof of global validity for the asymptotic approximations indicated above (see again Eqs. (61)-(63)). Such a proof seems unlikely at the present stage. In fact, let us assume for definiteness that the above asymptotic approximations are satisfied only at a prescribed initial time t_o by the initial $1-$body PDF $\rho_{1(o)}^{(N)}(\mathbf{x}_1)$ (being nevertheless uniformly fulfilled in the whole $1-$body phase-space Γ_1). In principle, there is no obvious reason warranting that their validity should be uniformly preserved in a global sense in the future, i.e., for all $t>t_o$. The conclusion is therefore that, while global validity is warranted both for the Master kinetic equation and the Master H-theorem for arbitrary initial conditions on the $1-$body PDF $\rho_{1(o)}^{(N)}(\mathbf{x}_1)$, this is not so in the case of the asymptotic Boltzmann equation and the corresponding asymptotic Boltzmann H-theorem.

8 - CONCLUSIONS

Motivated by mathematical/physical features of the original Boltzmann kinetic theory for hard-sphere systems which are intrinsically related to:

- *the inadequate functional setting adopted originally by Boltzmann for the kinetic equation bearing his name (Issue #1)*
- *the possible consequent violation of the same equation and the related Boltzmann H-theorem (Issue #2)*
- *the violation of the collision boundary conditions adopted in such a context (Issue #3)*
- *and, finally, the physical inconsistency of the Boltzmann-Grad limit (Issue #4)*

in this paper the problem of global existence has been reformulated in the context of the new "ab initio" approach for the Boltzmann-Sinai CDS recently developed in the context of Classical Statistical Mechanics [1, 2]. Such an approach has opened up a host of new exciting developments in kinetic theory, which are based on the construction of the Master kinetic equation [3–6].

In several respects the new theory, as well as the implications investigated in this paper, differ significantly from previous literature.

The main differences actually arise because of the non-asymptotic character of the new theory, i.e., the fact that it applies to arbitrary dense or rarefied systems for which the finite number and size of the constituent particles is accounted for [3]. In this paper basic consequences of the new theory have been investigated which concern the establishment of global existence theorems holding for such systems. First, the case of a generic solution of the $N-$body Liouville equation has been investigated. Then, an analogous theorem has been shown to hold also for factorized $N-$body PDFs. Thanks to the equivalence between Lagrangian and Eulerian forms of the Γ_N-phase-space Liouville equation, the latter result has been found to imply, in turn, a global existence theorem for the Master kinetic equation and for the corresponding Boltzmann-Shannon entropy (THM.1). Next the consequence of validity of the dilute-gas asymptotic approximation has then been investigated, and shown to warrant the global validity of an asymptotic kinetic equation and a related asymptotic H-theorem, respectively identified with the asymptotic Boltzmann equation and Boltzmann H-theorem.

Remarkably, all global existence theorems here determined apply when the underlying classical dynamical system is still finite. In other words, both the number of constituent particles N and the diameter of the hard-spheres σ are still finite, while being considered respectively $N \gg 1$ and $\sigma \sim O(\varepsilon^{1/2})$, suitable asymptotic approximations are introduced. Nevertheless, as far as the asymptotic Boltzmann equation and Boltzmann H-theorem, their global validity depends crucially on suitable asymptotic approximations. As pointed out above, such a prerequisite is non-trivial, since it depends on their uniform global validity. This implies that global validity of the asymptotic Boltzmann equation is not generally warranted for arbitrary initial conditions on the $1-$body PDF.

The present results are relevant, besides in mathematical research, for the physical applications of the new "ab initio" statistical theory, i.e., the Master kinetic equation. In particular, they provide the mandatory prerequisite for the investigation of the time-asymptotic properties of the same kinetic equation.

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APPENDIX: EXTENDED FUNCTIONAL SETTING

In the framework of the "ab initio" treatment of CSM [1–6] a suitable *extended functional setting* if assumed to hold for the $N-$body PDF$\rho^{(N)}(\mathbf{x},t)$. This requires to distinguish preliminarily suitable subsets of Γ_N which are necessary to prescribe its properties. In fact, each extended particle of the set S_N can only span the subset of configuration space Ω, here labeled as $\widehat{\Omega}$ and denoted here as *admissible configuration-space*, formed by the accessible configurations, i.e., which are permitted by the presence of the boundary surface and the remaining (extended) particles belonging to the same set S_N. For this purpose let us introduce the symbols

$$\Theta_i(\mathbf{r}) \equiv \Theta\left(\left|\mathbf{r}_i - \frac{\sigma}{2}\mathbf{n}_i\right| - \frac{\sigma}{2}\right) \prod_{j=1,i-1} \Theta\left(|\mathbf{r}_i - \mathbf{r}_j| - \sigma\right), \tag{74}$$

$$\overline{\Theta}_i(\mathbf{r}) \equiv \overline{\Theta}\left(\left|\mathbf{r}_i - \frac{\sigma}{2}\mathbf{n}_i\right| - \frac{\sigma}{2}\right) \prod_{j=1,i-1} \overline{\Theta}\left(|\mathbf{r}_i - \mathbf{r}_j| - \sigma\right), \tag{75}$$

with $\Theta(x) = \begin{cases} 1 & y \geq 0 \\ 0 & y < 0 \end{cases}$ and $\overline{\Theta}(y) = \begin{cases} 1 & y > 0 \\ 0 & y \leq 0 \end{cases}$ respectively the weak and strong Heaviside step function and $\mathbf{n}_i$ being the inward unit vector orthogonal to the boundary $\partial\Omega$ at the point of contact of the $i-$th hard sphere having center-of-mass position $\mathbf{r}_i$. Then introducing the ensemble weak and strong theta function $\Theta^{(N)}(\mathbf{r})$ and $\overline{\Theta}^{(N)}(\mathbf{r})$ defined respectively as

$$\Theta^{(N)}(\mathbf{r}) \equiv \prod_{i=1,N} \Theta_i(\mathbf{r}), \tag{76}$$

$$\overline{\Theta}^{(N)}(\mathbf{r}) \equiv \prod_{i=1,N} \overline{\Theta}_i(\mathbf{r}), \tag{77}$$

for definiteness, it is convenient to label as *collisionless* and *admissible subsets of* Γ_N the sets $\overline{\Gamma}_N$ and $\widehat{\Gamma}_N$ where the equations

$$\overline{\Theta}^{(N)}(\mathbf{r}) = 1, \tag{78}$$

or

$$\Theta^{(N)}(\mathbf{r}) = 1 \tag{79}$$

respectively hold. Hence the difference $\delta\Gamma_N \equiv \widehat{\Gamma}_N - \overline{\Gamma}_N$ necessarily identifies the *collision subset of* $\delta\Omega, \Gamma_N$, i.e., the corresponding subsets of Ω and Γ_N where collisions (unary, binary or multiple) for S_N occur.

Thus, in the *extended functional setting* for the *admissible functional class of solutions* of the Γ_N-phase-space Liouville equation, the $N-$body PDF$\rho^{(N)}(\mathbf{x},t)$ is assumed to coincide either with a stochastic PDF or with a distribution. In the first case this means that the same PDF fulfills the following properties:

1. is permutation symmetric, namely it is invariant w.r. to arbitrary particle permutations $(\mathbf{x}) \equiv (\mathbf{x}_1, ..., \mathbf{x}_N)$;
2. is a non-negative ordinary function in the whole extended phase space $\Gamma_N \times I$;
3. is a smooth function of class $C^{(k)}(\overline{\Gamma}_N \times I)$, with $k \geq 2$ in the open set $\overline{\Gamma}_N \times I$, with $\overline{\Gamma}_N$ being the collisionless subset of Γ_N defined by Eq. (78). Furthermore, $\rho^{(N)}(\mathbf{x},t)$ is required to admit for all $s = 1, N-1$ the *reduced* $s-$*body PDFs*

$$\rho_s^{(N)}(\mathbf{x}^{(s)},t) = F_s\left\{\rho^{(N)}(\overline{\mathbf{x}},t)\right\}, \tag{80}$$

   where $\mathbf{x}^{(s)} \equiv (\mathbf{x}_1, ..\mathbf{x}_s)$;
4. satisfies MCBC in collision subset of Γ_N, $\delta\Gamma_N$;
5. and $\rho_1^{(N)}(t)\rho_1^{(N)}(\mathbf{x}_1,t)$ admit respectively the phase-space and velocity moments

$$\int_{\Gamma_N} d\mathbf{x}\rho^{(N)}(\mathbf{x},t) = 1, \tag{81}$$

$$\int_{\Gamma_N} d\mathbf{v}_1 \mathbf{X}(\mathbf{x}_1,t)\rho_1^{(N)}(\mathbf{x}_1,t) = M_X(\mathbf{r}_1), \tag{82}$$

   where in the last integral $\mathbf{X}(\mathbf{x}_1, t) = 1, \mathbf{v}_1, v_1^2$.

In the case, instead, $\rho^{(N)}(\mathbf{x},t)$ is a distribution this means either that $\rho^{(N)}(\mathbf{x},t)$:

- coincides with the *$N-$body deterministic PDF*, i.e., $\rho^{(N)}(\mathbf{x},t) \equiv \rho_H^{(N)}(\mathbf{x},t)$, with $\rho_H^{(N)}(\mathbf{x},t)$ given by Eq. (5);
- is *a partially deterministic PDF*, namely it is of the form

$$\rho^{(N)}(\mathbf{x},t) = w^{(N)}(\mathbf{x},t)\delta(\xi(\mathbf{x})-\xi(\mathbf{x}(t))), \tag{83}$$

with $w^{(N)}(\mathbf{x},t)$ a suitable stochastic PDF and $\delta(\xi(\mathbf{x})-\xi(\mathbf{x}(t)) \equiv \prod\limits_{\mathbf{i=1,k}} \delta(\xi_\mathbf{i}(\mathbf{x})-\xi_\mathbf{i}(\mathbf{x}(t)))$. Here ξ denotes a $k-$component vector $\xi \equiv (\xi_i,..,\xi_k)$ and $\xi = \xi(\mathbf{x})$ a suitable smooth real vector function. In particular the corresponding $1-$body PDF will be taken of the form

$$\rho_1^{(N)}(\mathbf{x}_1,t) = w_1^{(N)}(\mathbf{x}_1,t)\delta(\xi_1(\mathbf{x}_1)-\xi_1(\mathbf{x}_1(t))). \tag{84}$$

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