On the Boltzmann-Grad Limit for the classical hard-spheres system

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Despite the progress achieved by kinetic theory, the search for possible exact kinetic equations remains elusive to date. This concerns, specifically, the issue of the validity of the conjecture proposed by Grad (Grad, 1972) and developed in a seminal work by Lanford (Lanford, 1974) that kinetic equations - such as the Boltzmann equation for a gas of classical hard spheres - might result exact in an appropriate asymptotic limit, usually denoted as Boltzmann-Grad limit. The Lanford conjecture has actually had a profound influence on the scientific community, giving rise to a whole line of original research in kinetic theory and mathematical physics. Nevertheless, certain aspects of the theory remain to be addressed and clarified. The purpose of this paper is to investigate the possible existence of the strong Boltzmann-Grad limit for the BBGKY hierarchy. Contrary to previous approaches in which the \( \text{w}^* \)-convergence was considered for the definition of the Boltzmann-Grad limit functions, based on their construction in terms of time-series expansions obtained from the BBGKY hierarchy, here we look for the possible existence of strong limit functions in the sense of local convergence in phase space. The result is based on the adoption of the Klimontovich approach to statistical mechanics, permitting the explicit representation of the \( s \)-body reduced distribution functions in terms of the Klimontovich probability density.

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1 - INTRODUCTION - FOUNDATIONS OF CKT

Basic issues concerning the foundations of classical kinetic theory (CKT) still remain unanswered. Since the criticism raised by Zermelo [2] on Boltzmann equation [1] the possibility of a rigorous construction of kinetic equations for classical gases has been the subject of investigations by many. In fact it is well known that Boltzmann himself obtained his famous equation using only physically plausible arguments, not first principles, i.e., the microscopic dynamics of the hard-sphere system. Despite the progress achieved by CKT in the last decades, its difficulty is notorious and is associated with the asymptotic character of kinetic equations, which potentially makes it hard - or even impossible - the construction of exact kinetic equations for many systems, in particular for classical systems of interacting hard spheres. As such, the investigation of the rigorous of CKT represents a challenge both for mathematical analysis and mathematical physics alike. Its importance for gas dynamics and classical hydrodynamics goes beyond the academic interest. One such problem is posed by the possible existence of exact kinetic equations obtained in the so-called Boltzmann-Grad (B-G) limit, which should apply to infinite classical systems of interacting particles, provided the microscopic phase-space distribution function (PSDF) satisfies physical constraints and functional settings to be properly defined. The goal of this investigation is to propose a novel approach to CKT, pertaining to hard-sphere systems, based on the investigation of the properties of the so-called limit functions which are obtained for such systems in the B-G limit. In particular, we wish to investigate the limit functions which enter the BBGKY and prove that - contrary to common belief - they do not generally belong to the functional class of the solutions of the asymptotic Boltzmann hierarchy. This means, in particular, that in the case of smooth and hard sphere systems, the limit functions do not generally satisfy the exact Boltzmann kinetic equation, although the explicit construction of asymptotic solutions for the BBGKY hierarchy can be achieved based on the determination of suitable weakly-convergent sequences.

1a - Basic motivations: 'ab initio' approaches

Classical statistical mechanics, and in particular kinetic theory represents, is a sense, one of the unsolved problems of classical mechanics. In fact, although the microscopic statistical description (MSD) of classical dynamical systems formed by \( N \)-body systems is well known, a complete knowledge of their solutions is generally not achievable. From the mathematical viewpoint it provides an example of axiomatic approach following from first principles and as such it must be considered as an 'ab initio' formulation. Two equivalent treatments of MSD are known, which are based respectively on the introduction of a phase-space distribution function (PSDF) either on the \( N \)-body phase-space \( \Gamma_N \) or, respectively, on the 1-particle phase-space \( \Gamma_1 \). In the \( \Gamma_N \)-approach the PSDF is the so-called microscopic PSDF \( f_N \). It follows that \( f_N \) obeys the Liouville equation, whose characteristics are simply the phase-space trajectories of the same
dynamical system, to be identified with a classical $N$-body system $\overline{3}$. This equation is equivalent to a hierarchy of equations (the so-called BBGKY hierarchy) for a suitable set of $s$-particles distribution functions $f_s^{(N)}$, obtained letting $s = 1, \ldots, N-1$, which are uniquely related to the corresponding PSDF. On the other hand, in the $\Gamma_1$-approach the PSDF (the Klimontovich probability density $k^{(N)}$, defined in the $\Gamma_1$-space) evolves in time by means of the Klimontovich equation $[4]$. Also for this equation the characteristics are just the phase-space trajectories of the $N$-body system, this time - however - projected on the $\Gamma_1$-space. Therefore, in both cases it is actually necessary to determine the phase-space trajectories of all the particle. Hence, for classical systems characterized by a large number of particles ($N \gg 1$), the computational complexity (of this problem) is expected to prevent, in general, any direct calculation of the time-evolution either of the $N$-body or any of the the $s$-body distributions. This has justified the constant efforts placed so-far for the search of 'reduced' statistical descriptions, of which kinetic theory (KT) is just an example. This is intended in order to achieve efficient statistical descriptions especially suitable for complex dynamical systems, including both gases and plasmas. Precisely, the primary goal of KT is the search of statistical descriptions, either exact or in some sense approximate, whereby the whole dynamical system is associated only to the one-particle kinetic distribution function ($f_1$) defined on the one-particle phase-space $\Gamma_1$, without requiring the knowledge of the dynamics of the whole dynamical system. As a consequence in KT-descriptions the evolution equation of the kinetic distribution function, to be denoted as kinetic equation, is necessarily assumed to depend functionally, in some suitable sense, only on the same distribution function and the one-particle dynamics. In particular, one of the most successful developments of KT is doubtless related to the so-called 'ab initio' approaches. These are to be intended (in contrast to heuristic or model equations) as the KT’s which are obtained deductively - by suitable approximation schemes and assumptions - from the corresponding exact MSD. In traditional approaches usually KT is obtained adopting the $\Gamma_N$-approach to MSD $\overline{3} \overline{8} \overline{12}$. However, also the Klimontovich method (based on the $\Gamma_1$-approach) can be used $[4]$, since it is completely equivalent to that based on the $\Gamma_N$-approach $\overline{2} \overline{8}$. In all cases KT’s have the goal of determining the evolution of suitable fluid fields, associated to prescribed fluids, which are expressed as *velocity moments of the kinetic distribution function* $f_1$ and satisfy an appropriate set of fluid equations, generally not closed, which follow from the relevant kinetic equation. 'Ab initio' kinetic theories are - however - usually asymptotic in character. Namely, kinetic equations are typically satisfied only in an approximate (and asymptotic) sense and in a finite time interval, under suitable assumptions. These require in particular that $f_N$ (and all $f_s$, for $s = 1, N-1$) must belong to a suitable functional class (here denoted as $\{f_N\}$) so that $f_N$ as well as the related $s$-particle distribution functions $f_s^{(N)}$ satisfy appropriate initial and boundary conditions.

1b - Asymptotic kinetic theories

A well-known asymptotic kinetic equation of this type is provided by the Boltzmann kinetic equation for a classical gas formed by $N$ smooth rigid spheres of diameter $d$ (Grad,1958 $\overline{3}$), which is obtained from the exact equation of the BBGKY hierarchy for the one-particle kinetic distribution, i.e.,

$$F_1(x_1,t)f_1^{(N)}(x_1,t) = d^2(N-1)\left\{C_1f_2^{(N)}\right\}_{(x_1,t)}, \quad (1)$$

where $F_1$ and $C_1f_2^{(N)}$ are respectively the free-streaming operator $F_1(x_1,t)=\frac{dv_1}{\rho_1}+\frac{dv}{\rho_2}$ and the BBGKY collision operator $C_1\rho_2^{(N)} = \int d\Sigma_2\rho_2^{(N)}v_{12}\cdot n_{12}$, containing the integration on velocity and the solid angle $d\Sigma_2$ of particle 2, and the notation is standard $\overline{3} \overline{8} \overline{12}$. Thus $x_1=(r_1, v_1)$ is the Newtonian state of particle 1, $n_{12}$ is unit vector $n_{12}=r_{12}/|r_{12}|$, while $v_{12}=v_1-v_2$ and $r_{12}=r_1-r_2$ are respectively the relative velocities and position vectors of particles 1 and 2. For definiteness, in the remainder we adopt a dimensionless notation whereby all relevant functions (in particular, the Newtonian particle state $x_1=(r_1, v_1)$, the time $t$, the particle diameter $d$ and the volume of the configuration space $V$) are considered non-dimensional. Eq. (1) can also be written in the integral form

$$f_1^{(N)}(x_1(t),t) = f_1^{(N)}(x_{10},t_0) +$$

$$+ d^2(N-1) \int_{t_0}^{t} dt' \left\{C_1f_2^{(N)}\right\}_{(x_i(t'),t')}, \quad (2)$$

by integrating the previous equation along the Lagrangian characteristics $x_i(t)$. The equation can be iterated by representing in a similar way the $s$-particle joint probability densities $f_s^{(N)}$ for $s = 2, 3, \ldots$, etc., obtained integrating the corresponding equations of the BBGKY hierarchy. The transition from the 1-particle equation (1) can be obtained by adopting a suitable asymptotic approximation and appropriate assumptions on the joint probability densities $\overline{3} \overline{8}$. These require, in particular, the introduction of the so-called rarefied gas ordering (RG ordering) for the relevant physical parameters, to be intended both in a global and local sense. More precisely, by imposing that $\varepsilon = 1/N$ is an infinitesimal, the particle diameter $d$, the volume $V$ of the configuration space ($\Omega$) and the particle mass $m$ must be suitably ordered in terms of $\varepsilon$. Thus, the global ordering is obtained requiring that $d$ and $m$ are respectively infinitesimals of
order $\varepsilon^{1/2}$ and $\varepsilon$, whereas the volume of the configuration space is taken of order $O(1)$ (Grad, 1958 [3]). This implies that average volume fraction $\tilde{\eta} \equiv 4\pi N d^3/3V$ results necessarily an infinitesimal of order $\varepsilon^{1/2}$. In addition, to assure that the gas is rarefied everywhere in $\Omega$, the local volume fraction $\eta(r,t) \equiv 4\pi n(r,t)d^3/3V$ must be assumed of order $\varepsilon^{1/2}$ everywhere in $\Omega \times I_{o1}$ (local ordering). Here $I_{o1}$ is the time interval $I_{o1} = [t_o, t_1]$, with $\Delta t = t_1 - t_o$ defined so that $\Delta t \sim O(1)$ and $n(r,t)$ is the local number density. Thus, the local ordering prevents the number density from becoming so large for $\eta(r,t)$ to be locally finite, i.e., of order $O(1)$. It is well-known, in fact, that if $\eta(r,t)$ becomes locally of order $O(1)$, particle correlations (in particular two-particle correlations) may become non-negligible also on a larger scale [3, 6, 7]. These correlations, which are not generally expected to decay rapidly in time [8], can be long-range in character [9]. Instead, in validity of the RG ordering - and in particular imposing of the local ordering indicated above - the following conditions are assumed to be satisfied uniformly in phase-space and at least in a finite time interval $I = [t_o, t_1]$, with $\Delta t = t_1 - t_o$ such that $\Delta t \sim O(1)$:

- Assumption #1 - in $\Gamma_s \times I_{o1}$, the approximate (i.e., asymptotic) joint probability densities $f_s(\varepsilon, x_i, t) = \prod_{i=1,s} f_1(\varepsilon, x_i, t) [1 + \Theta(t - t_o)\varepsilon^{\alpha}]$ is satisfied identically for any $s \in N$ such that $s/N$ is an infinitesimal of order $\varepsilon$. Here $f_1(\varepsilon, x_i, t)$ is the one-particle probability density which satisfies the asymptotic Boltzmann equation

$$F_1(r_1, v_1, t) f_1(\varepsilon, t) = d^2 NC_1 f_2(\varepsilon),$$

and $\Theta(t - t_o)$ is the Heaviside theta function which vanishes for $t = t_o$.

If the RG ordering and the previous assumptions hold locally (i.e., in the whole phase-space $\Gamma_1$ and at least in a finite time interval $I_{o1} = [t_o, t_1]$), the Boltzmann equation (4) is expected to be locally valid in the same domain [10, 21, 22] at least in an asymptotic sense.

Even if the rigorous proof of the global validity of the Boltzmann equation for arbitrary initial and boundary conditions has yet to be reached, its success in providing extremely accurate predictions for the dynamics of rarefied gases and plasmas is well known (see for example, Cercignani, 1969 [8], Frieman, 1974 [10]).

1c - The Boltzmann-Grad limit and the Lanford conjecture

Nevertheless, basic issues remain to be clarified regarding the rigorous theoretical foundations of kinetic theory. Following the conjecture suggested originally by Grad (Grad, 1972 [5]; see also Grad, 1972 [2] and Frieman, 1974 [11]), that the Boltzmann kinetic equation for a gas of classical hard spheres - may result exact. A basic difficulty is to properly formulate the related mathematical problem and to ascertain in a rigorous way the possible validity of such a type of statements. One such problem refers in particular to the search of possible exact kinetic equations and, specifically, the conjecture (here denoted as Lanford conjecture) proposed by Lanford in a seminal paper (Lanford, 1974 [3]; see also Grad, 1972 [5] and Frieman, 1974 [10]), that the Boltzmann kinetic equation for a gas of classical hard spheres might result exact in an appropriate asymptotic limit, denoted as Boltzmann-Grad (B-G) limit.

The B-G limit is customarily intended as the limiting "regime" where the total number of particles $N$ goes to infinity, while the configuration-space volume $V$ remains constant, the particle diameter $d$ goes to zero in such a way that $Nd^2$ approaches a finite non-zero constant and the average mass density $Nm/V = M/V$ remains finite (Grad, 1972 [3]; Lanford, 1974 [9]), i.e., there results:

$$\frac{1}{N}, d, m \rightarrow 0,$$

$$\frac{N d^2}{V} \rightarrow k_1,$$

$$\frac{M}{V} \rightarrow k_2,$$

where $k_i$ (for $i = 1, 2$) are prescribed non-vanishing positive and finite constants. In the case of plasmas further analogous requirements are placed on the total electric charge and current carried by each particle species [10, 26]. In the original Lanford formulation, it was conjectured that, subject to suitable initial and regularity conditions, the one-particle probability density determined by the integral equation [27] converges weakly, in the sense of weak * convergence, to a limit function $f_{w1}(x_1, t) = L_{w1} f_1^{(N)}(x_1, t)$, $L_{w1}$ denoting an appropriate operator, to be denoted as weak B-G limit operator and $f_{w1}(x_1, t)$ the solution of the equation [stemming from Eq. (2)]

$$f_{w1}(x_1, t) = f_{w1}(x_1, t_0) +$$

$$+ V k_1 \int_{t_0}^{t} dt' L_{w1} \left\{ C_1 f_2^{(N)} \right\}(x_1(t'), t').$$

In this meaning the conjecture was actually proven true by Lanford, at least in a partial sense, namely for a time interval which has an amplitude not exceeding one fifth
of the mean free path measured from an initial time \( t_0 \) (Lanford Theorem). The proof, first presented in his work on the B-G limit (Lanford, 1974 [9]) under the assumption of factorization at the initial time (i.e., Eq. [9] taken at \( t = t_0 \), while letting \( \varepsilon \to 0 \)), was actually reached by proving the convergence, in the sense of weak *-convergence, of the limit time-series solution [9]. Obviously, this result does not suffice to justify possible meaningful physical applications. Nevertheless, the conjecture has actually had a profound influence on the scientific community, giving rise to a whole line of original research in kinetic theory and mathematical physics. In particular, the proof has been extended to more general situations [19, 21, 22, 23]. Nevertheless, despite the progress achieved by kinetic theory, the issue of existence of the B-G limit remains, however, open to date. Despite the significant number of theoretical papers appeared in the literature in the last three decades, the issue of the validity of the Boltzmann equation in the B-G limit is generally insufficient to specify uniquely the B-G limit. It is obvious, in fact, that in principle the B-G limit may be taken locally in arbitrary ways, so that the (strong) B-G 1-particle limit function is not a solution of the Boltzmann equation.

Here we want to investigate a basic issue - preliminary w.r. to the treatment of the Boltzmann equation - namely the validity of the Lanford conjecture for the BBGKY hierarchy itself, to be intended in the sense of the strong B-G limit, here denoted as strong Lanford conjecture. The conjecture requires, that there exists a strong B-G limit operator \( L^* \) which, applied to the equations of the BBGKY hierarchy for the \( s \)-particle joint probability densities \( f^{(N)}_s \), delivers the corresponding equations of the Boltzmann hierarchy for the corresponding limit functions \( f_s = L^* f^{(N)}_s \) that a suitable limit-hierarchy must exist (to be denoted as the Boltzmann hierarchy) for suitable \( s \)-particle limit functions \( f_s \equiv L^* f^{(N)}_s \) (for \( s \in \mathbb{N} \)). In particular in the case of the BBGKY equation for one-particle probability density

\[
F_1 f^{(N)}_1 = d^2 (N - 1) C_1 f^{(N)}_2,
\]

applying the operator \( L^* \) to both sides it should result identically the (exact) equation of the Boltzmann hierarchy

\[
F_1 f_1 = d^2 N C_1 f_2.
\]

This means that the strong limit functions \( f_s = L^* f^{(N)}_s \) (for \( s = 1, 2 \)) should have the property that:

- a) the limit function \( f_1 = L^* f^{(N)}_1 \) should belong to the functional class of the solutions of the Boltzmann hierarchy;
- b) it should result identically

\[
[L^*, F_1] f^{(N)}_1(x_1, t) \equiv 0,
\]

where \( [L^*, F_1] \) denotes the commutator \( [L^*, F_1] = L^* F_1 - F_1 L^* \). This means that
the operators $L^*$ and $F_1$ should commute when acting on the one-particle probability density;

- c) and finally the following limit:

$$L^*d^2(N-1)C_1f^{(N)}_1 = d^2NC_1L^*f^{(N)}_2$$

should hold.

Main goal of the investigation is to analyze the possible validity of the strong Lanford conjecture here proposed and in particular whether properties a)-c) are generally fulfilled or not, in other words, whether the strong B-G limit function $f_1 = L^*f^{(N)}_1$ may belong or not to the functional class of the solutions of the corresponding equation of the Boltzmann hierarchy.

The possible solution of this problem goes beyond the academic interest. In fact, not only it represents a difficult theoretical problem, but it is related to the very foundations of statistical mechanics. As such, its investigation represents a challenge both for mathematical analysis and for theoretical physics. The possible solution of the riddle posed by the strong Lanford conjecture provides, in fact, a new interesting starting point for theoretical research in kinetic theory. This paper will analyze for this purpose the classical model based on a gas of hard-smooth spheres. The approach is based on the adoption of the Klimontovich approach to statistical mechanics, permitting the explicit representation of the $s$-body reduced distribution functions in term of the Klimontovich probability density.

2 - MSD APPROACH FOR THE HARD-SPHERE SYSTEM IN THE $\Gamma_1$-PHASE-SPACE

Let us consider the time evolution of a system $(S_N)$ of $N$ identical smooth spheres. The particles are assumed of diameter $d$, mass $m$ and immersed in a compact connected configuration domain $\Omega \subset \mathbb{R}^3$, with prescribed fixed boundary $\partial \Omega$ represented by a smooth regular surface $\mathbb{R}^3$. In the sequel particles are assumed to be subject only to binary and unary elastic collisions. Both occur when the boundaries of the particles and/or $\partial \Omega$ come into mutual contact in such a way that the colliding boundaries, before collision, have a non-vanishing relative velocity. Multiple collisions - i.e., simultaneous collisions between particles and/or $\partial \Omega$, by assumption, are considered as sequences of binary and/or unary collisions. For definiteness, we shall assume all particles to be 'hard', i.e., such that their boundaries are rigid and furthermore that each particle can come into contact with $\partial \Omega$ only in a single point. This condition is satisfied, for example, if $\partial \Omega$ is identified with a spherical surface (of radius $R_0$). In such a case only a subset of admissible configurations of $\Omega$ is actually permitted. This is defined as the set $\Omega = \{ r : r \in \Omega, \Theta_i(r, \xi(t), t) = 1, \forall i = 1, N \}$, where $\Theta_i(r, \xi(t), t)$ is the occupation function for the $i$-th particle, $\Theta_i(r, \xi(t), t) = 1 - \sum_{j=1,N \atop i \neq j} \Theta(d - |r - r_j(t)|) - \Theta(d/2 - |r - r_W|)$. Here $r_W$ is a position vector defining an arbitrary point of the boundary $\partial \Omega$, $\xi(t)$ denotes the $N$-particle configuration vector $\xi(t) = \{ r_1(t), ..., r_N(t) \}$, while $\Theta(x)$ is the so-called strong Heaviside step function i.e., $\Theta(x) = 1, 0$ if $x > 0$, $x \leq 0$. We stress that in the definition of all the occupation functions (both $\Theta_i$ and $\Theta$, given below) the configuration vector $\xi(t)$ is defined in such a way that the position vectors $r_1(t), ..., r_N(t)$ are always considered mutually admissible. This means in particular that for all $i, j = 1, N$ (with $i \neq j$) it must result in $|r_i(t) - r_j(t)| \geq d$. One can define in a similar way also the subset of $\Omega$ (to be denoted as $\Omega$) in which no interactions occur (for all particle of $S_N$) as well as the corresponding occupation function, to be denoted as strong occupation function. The latter reads for the $i$-th particle:

$$\Theta_i(r, \xi(t), t) \equiv 1 - \sum_{j=1,N \atop i \neq j} \Theta(d - |r - r_j(t)|) - \Theta(d/2 - |r - r_W|),$$

where $\Theta(x)$ is the strong Heaviside step function i.e., $\Theta(x) = 1, 0$ if $x > 0$, $x \leq 0$. It follows that the set $\Omega$ is simply the subset of $\Omega$ in which the equations $\Theta_i(r, \xi(t), t) = 1$ are satisfied identically for all particles, i.e., for all $i = 1, N$. Moreover, by assumption, particles are 'smooth'. This means that they undergo only interactions (collisions) which conserve the angular momenta of all particles. Hence, the state of $S_N$ is uniquely defined by ensemble of states $x(t) = \{ x_1(t), ..., x_N(t) \} \equiv \xi(t), \eta(t)$, where $x_i(t)$ for $i = 1, N$ represents the state of each particle defined by the vector $x_i(t) = \{ r_i(t), v_i(t) \}$, $r_i(t)$ and $v_i(t)$ denoting the positions and velocities of the centers of each sphere. Thus, $\eta(t) \equiv \{ v_1(t), ..., v_N(t) \}$ while each vector $x_i(t)$ (for $i = 1, N$) spans the one-particle admissible phase-space $\Gamma_1(i) = \Omega \times \mathbb{R}^3$. We notice that in a similar way it is possible to define admissible and forbidden sub-domains in the $N$-particle configuration-space $\Omega^N$ and in the corresponding phase-space $\Gamma_N = \Omega^N \times \mathbb{R}^3N$. In particular, we denote by $\Gamma_s$ (respectively $\Gamma_s$) the admissible subsets of $\Gamma_N$ ($\Gamma_s$) in which the configurations of all $N$ particles (respectively of the first $s$ particles) are all admissible and $\Gamma_N = \Gamma_N - \Gamma_s$ ($\Gamma_s = \Gamma_s - \Gamma_s$) its complementary set, denoting the forbidden sub-domain of $\Gamma_N$ ($\Gamma_s$).

Regarding particle dynamics, the motion of each ($i$-th) particle of $S_N$ is assumed inertial in any open subset $\left[ t_k^{(i)} , t_{k+1}^{(i)} \right]$ of $I$ not containing collision events for the same particle (the time interval between two successive collision events occurring). Finally, at an arbitrary collision time for the same particle ($t_c^{(i)}$), the phase-flow is defined respectively, for binary and unary interactions, by
the elastic two- and one-particle collision laws [3], which uniquely relate its states before \([x_i^-(t_o)]\) and after collision \([x_i^+(t)]\). As a consequence, the mapping provided by the phase-flow between an arbitrary admissible initial state \(x(t_o) = x_o\), with \(x_o = \{x_{1o}, \ldots, x_{No}\}\), and its image at an arbitrary time \(t \in I \equiv \mathbb{R}\), \(x(t) = \chi(x_o, t - t_o) \in \mathbb{T}_N\) is manifestly defined globally in \(\Gamma_N \times I\).

The microscopic statistical description of \(S_N\) adopting the \(\Gamma_N\)-phase-space description - and based on the introduction of the PSPD \(f_N(x,t)\) in \(\Gamma_N\) - is well-known [8, 12]. The relevant mathematical framework is recalled in the Appendix (see in particular Theorem 1).

The MSD for \(S_N\) on the phase-space \(\Gamma_1\) can, instead, be achieved by introducing the Klimontovich probability density for \(S_N\) on the same phase-space. Following the Klimontovich approach [3], this is defined as a probability distribution on \(\Gamma_1\) which is assumed as non-vanishing only along the subsets of the trajectories of the particles of \(S_N\) system (all mapped on the phase-space \(\Gamma_1 \equiv \Omega \times \mathbb{R}^3\) where all particles of \(S_N\) are not subject to interactions, i.e., in the subset \(\Gamma_1 = \Omega \times \mathbb{R}^3\). Hence, the Klimontovich probability density necessarily takes the form:

\[
k^{(N)}(y,t) = \frac{1}{N} \sum_{i=1,N} \delta(y - x_i(t))\Theta_i(r, \xi(t), t)\tag{14}
\]

where \(\Theta_i(r, t)\) is the occupation function defined by Eq. (13) and \(y = (r, v) \in \Gamma_1\). Hence, it follows that \(k^{(N)}(y,t)\) in \(\Gamma_1\) satisfies identically the \(\Gamma_1\)-space Liouville equation:

\[
\left(\frac{\partial}{\partial t} + v \cdot \nabla\right)k^{(N)}(y,t) = 0. 
\tag{15}
\]

Then the following theorem applies:

**Theorem 2 - \(\Gamma_1\)-MSD for \(S_N\)**

Let us assume that for \(S_N\) the microscopic probability density \(f_N(x,t)\) satisfies assumptions of THM.1 (see Appendix). Then it follows that:

A) in \(\Gamma_1 \times I\) (for any \(y \equiv (r, v) \in \Gamma_1\) and \(t \in I \subseteq \mathbb{R}\) the 1-particle probability density \(f_1^{(N)}(y,t)\) admits the integral representation in terms of the initial microscopic probability density \(f_N(x_o, t_o)\):

\[
f_1^{(N)}(y,t) = \int_{\Gamma_N} dx_o f_N(x_o,t_o) \frac{1}{N} \sum_{i=1,N} \delta(y - x_i(x_o,t-t_o))\Theta_i(r, \xi(t), t), \tag{16}
\]

where \(\Theta_i(r, \xi(t), t)\) is the strong occupation number [13], with \(\xi(t) \equiv \{r_1(x_o,t-t_o), \ldots, r_N(x_o,t-t_o)\}\);

B) in terms of \(f_N(x,t)\) the 1-particle probability density reads identically in \(\Gamma_1 \times I\) as :

\[
f_1^{(N)}(y,t) = \int_{\Gamma_N} dx_o f_N(x_o,t_o) \frac{1}{N} \sum_{i=1,N} \delta(y - x_i)\Theta_i^*(r,t), \tag{17}
\]

where \(\Theta_i^*(r, \xi, t)\)

\[
\Theta_i^*(r, \xi, t) \equiv 1 - \sum_{j=1,N; j \neq i} \Theta(d - |r - r_j|) - \Theta(d/2 - |r - r_W|), \tag{18}
\]

and \(\xi \equiv \{r_1, \ldots, r_N\}\).

Proof

The proof follows by noting:

A) first, that Eqs. (16) and (17) mutually imply each other thanks to the validity of Liouville equation for \(f_N(x,t)\) [see Eq. (38) in the Appendix] in the sub-domain of \(\Gamma_N\) where no interactions (unary or binary) occur;

B) second, from Eq. (17) there follows, in particular, for \(f_1^{(N)}(y,t)\) the identity

\[
f_1^{(N)}(y,t) = \int_{\Gamma_2} dx_1 dx_2 f_2(x_1, x_2) \delta(y - x_1)\Theta_1^*(r, \xi, t), \tag{19}
\]

which immediately implies Eq. (9) for \(s = 1\). c.v.d.

### 3 - A REPRESENTATION OF \(f_1^{(N)}(y,t)\) BASED ON FUNCTIONAL CONTINUATION

We notice that the proof of THM.1 can also be reached by introducing a functional continuation - denoted as \(f_N^c(x,t)\) - of \(f_N(x,t)\) in the open subset \((\Gamma_N^c)\) of the forbidden sub-domain \(\Gamma_N\), where the particles of \(S_N\) are not interacting with the boundary \(\partial\Omega\). The only minimal requirement to be imposed on \(f_N^c(x,t)\) is that it results continuous on the boundary set between \(\Gamma_N^c\) and \(\Gamma_N\), \(\delta\Gamma_N^c \cap \partial\mathbb{T}_N\) (A). However, due to the freedom in its definition it is always possible to require also that:

- B) \(f_N^c(x,t)\) is non-negative in the whole set \(\Gamma_N \times I\) and strictly positive in \(\Gamma_N^c \times I\);

- C) \(f_N^c(x,t)\) is invariant with respect to arbitrary permutations of like particles;

- D) in the forbidden sub-domain \(\Gamma_N\) \(f_N^c(x,t)\) satisfies the differential Liouville equation

\[
\frac{\partial}{\partial t}f_N^c(x,t) + \sum_{i=1,N} v_i \cdot \nabla_i f_N^c(x,t) = 0. \tag{20}
\]

It is obvious that Eq. (16) remains valid even if \(f_N(x,t)\) is replaced by the an arbitrary functional continuation satisfying these assumptions (A-D). This permits us to reach the following integral representation for \(f_1^{(N)}(y,t)\):

\[
\int_{\Gamma_N} dx_o f_N(x_o,t_o) \frac{1}{N} \sum_{i=1,N} \delta(y - x_i)\Theta_i^*(r,t).
\]
Corollary 1 of Thm. 2 - Integral representation for $f_1^{(N)}(y, t)$

In terms of the functional continuation $f_2^N(x, t)$ there results identically in $\Gamma_1 \times I$ (for any $y \equiv (r, v) \in \Gamma_1$ and $t \in I \subseteq \mathbb{R}$):

$$f_1^{(N)}(y, t) = I_1^{(N)} - I_2^{(N)}$$

(21)

where $I_1^{(N)}$, $I_2^{(N)}$ are the phase-space integrals

$$I_1^{(N)} = \int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t)$$

(22)

$$I_2^{(N)} = (N - 1) \int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t) \Theta(d - |r - r_2|)$$

(23)

and the notation

$$f_2^{(N)}(y, x_2, t) \equiv \int_{\Gamma_N} dx f_N(x, t) \delta(y - x_1)$$

(24)

has been introduced.

Proof

In fact in terms of $f_N^x(x, t)$ Eq. (17) reads

$$f_1^{(N)}(y, t) = \int_{\Gamma_N} dx f_N^x(x, t) \frac{1}{N} \sum_{i=1, N} \delta(y - x_i) -$$

$$- \int_{\Gamma_N} dx f_N^x(x, t) \frac{1}{N} \sum_{i=1, N} \delta(y - x_i) \sum_{j=1, N} \Theta(d - |r - r_j|)$$

(25)

which delivers, upon imposing condition B,

$$f_1^{(N)}(y, t) = \int_{\Gamma_N} dx f_N^x(x, t) \delta(y - x_1) -$$

$$-(N - 1) \int_{\Gamma_N} dx f_N^x(x, t) \delta(y - x_1) \Theta(d - |r - r_2|).$$

(26)

This equation reduces to (21) by introducing the notation given above [see Eq. (22)]. c.v.d.

We remark, furthermore that the following additional proposition holds:

**Corollary 2 (THM. 2) - Inequality for $I_2^{(N)}$**

In validity of THM. 2, the phase-space integral $I_1^{(N)}$ satisfies for all $(r, v, t) \in \Gamma_1 \times I$ the homogeneous equation

$$F_1(r, v, t) I_1^{(N)} = 0,$$

(27)

where $k_{sup}$ is a suitable strictly positive real constant independent of $N$.

Proof.

The proof is immediate thanks to Eq. (20) which, by assumption, is satisfied by $f_N^x(x, t)$.

4 - THE STRONG B-G LIMIT FOR $S_N$

Let us now show how theorem 2 permits us to determine the strong B-G limit of $f_1^{(N)}$, $f_1(y, t) \equiv L^* f_1^{(N)}$. Here $L^*$ denotes the strong B-G limit operator which is defined in the sense of local convergence for ordinary functions defined in phase-space and is obtained letting $N \to \infty$ while requiring $d = c/N^{1/2}$, with $c$ a non-vanishing finite constant independent of $N$. In the sequel the limit operator $L^*$ acts on $f_1^{(N)}$ or $f_2^{(N)}$, both considered defined point-wise in suitable domains. In particular, the $L^*$ coincides with the ordinary limit operator when acting on an arbitrary real function of the parameters $N$ and $d$. Let us now assume that both $f_1^{(N)}(y, t)$ and $f_1^{(N)}(y, t)$ are bounded, i.e., $\sup(f_1), \sup(f_1^*) < \infty$.

In such a case the following Lemma holds:

**Lemma (to THM. 3) - Inequality and B-G limit for $I_2^{(N)}$**

In validity of THM. 2, let us assume that at least in a finite time interval $I_{a1} = [t_a, t_1] \subseteq I$ and in $\Gamma_1^{a,}$, $f_2^{(N)}(y, x_2, t)$ can be defined so that everywhere in $\Gamma_1 \times I_{a1}$:

a) the limit functions $f_s \equiv L^* f_s^{(N)}$ and $f_s^* \equiv L^* f_s^{(N)}$ exist for $s = 1, 2$ at least in $\Gamma_1 \times I_{a1}$;

b) $f_1^{(N)}$ and $f_1^{(N)}$ (for arbitrary $N \in \mathbb{N}$) as well as $f_s$ and $f_s^*$ (for $s = 1, 2$) are, bounded ordinary functions defined at least in $\Gamma_1 \times I_{a1}$;

c) the phase-space integrals :

$$\int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t) \Theta(d - |r - r_2|)$$

(25)

for any $N \in \mathbb{N}$

and $L^*$

$$\int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t) \Theta(d - |r - r_2|)$$

are bounded;

d) the functions: $f_1^{(N)}(y, t)$ (for any $N \in \mathbb{N}$) and $f_1^{(N)}(y, t) \equiv L^* f_1^{(N)}(y, t) \equiv L^* \int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t)$ are strictly positive,

Then it follows that in $\Gamma_1 \times I_{a1}$:

L-I) for any finite $N \in \mathbb{N}$ the phase-space integral $I_2^{(N)}$ can be majorized as follows

$$I_2^{(N)} \leq (N - 1) \int_{\Gamma_1(2)} dx_2 f_2^{(N)}(y, x_2, t) \Theta(d - |r - r_2|).$$

(28)

where $k_{sup}$ is a suitable strictly positive real constant independent of $N$; L-II) uniformly in $\Gamma_1 \times I_{a1}$ there holds:

$$L^* I_2^{(N)} = 0.$$

(29)

Proof
The proof is immediate. In fact, due to assumptions a) and b), together with the strict positivity of $f_1^{s(N)}(y,t)$ (assumption d), we can always require that in a finite time interval $I_{o1} = [t_{o1}, t] \leq I$ there results

$$
\int_{\Gamma_{1(2)}} d\mathbf{x}_2 f_2^{s(N)}(\mathbf{y}, \mathbf{x}_2, t) \Theta(d - |\mathbf{r} - \mathbf{r}_2|) \leq (30)
$$

$$
\leq \frac{d^3}{V} k_{\text{sup}} \int_{\Gamma_{1(2)}} d\mathbf{x}_2 f_2^{s(N)}(\mathbf{y}, \mathbf{x}_2, t) = \frac{d^3}{V} k_{\text{sup}} f_1^{s(N)}(\mathbf{y}, t),
$$

where $k_{\text{sup}}$ is a suitable strictly positive real constant. In particular, since the inequality must hold for any $N > 1$, $k_{\text{sup}}$ can always be chosen as independent of $N$. This implies the inequality (28).

L-II To prove Eq. (30) let us invoke the majorization (29) which implies

$$
L^* I_{2(N)}^{(2)} \leq L^* \left\{ (N-1) \frac{d^3}{V} k_{\text{sup}} f_1^{s(N)}(\mathbf{y}, t) \right\},
$$

(31)

Due to assumption c) $\sup (f_1(\mathbf{y}, t)) < +\infty$ while $k_{\text{sup}}$ is independent of $N$. It follows

$$
L^* I_{2(N)} \leq k_{\text{sup}} \sup (f_1(\mathbf{y}, t)) L^* \left\{ (N-1) d^3 \right\}.
$$

(32)

Hence, since in the B-G limit by definition $L^* \{(N-1)d^3\} = 0$, this means that $L^* I_{2(N)}^{(2)}$ is identically zero in the set $\Gamma_1 \times I_{o1}$. c.v.d.

We remark that to satisfy the condition of strict positivity here imposed on $f_1^{s(N)}(\mathbf{y}, t)$ and $f_1(\mathbf{y}, t)$ [see assumption d) in the Lemma] it is actually sufficient to require that $f_1^{s(N)}(\mathbf{y}, t)$ and its limit function $f_1(\mathbf{y}, t)$ are strictly positive in $\Gamma_1 \times I_{o1}$. This is because by definition $f_1^{s(N)}(\mathbf{y}, t) \geq f_1(\mathbf{y}, t)$, while one can prove that $f_1(\mathbf{y}, t) = f_1(\mathbf{y}, t)$ (see below). Then the following theorem has the flavor of:

**Theorem 3 - Strong B-G limit for $S_N$**

In validity of THM.2 and the Lemma, assuming that the limit functions $f_1(y, t)$ and $f_1^{s}(y, t)$ exist and are bounded at least in the space $\Gamma_1 \times I_{o1}$, there it follows for $S_N$ that:

T-1) uniformly in $\Gamma_1 \times I_{o1}$, the strong B-G limit function $f_1(y, t) \equiv L^* f_1^{s(N)}(y, t)$ reads

$$
f_1(y, t) = f_1^{s}(y, t); \quad (33)
$$

T-1) $f_1(y, t)$ satisfies identically the homogeneous equation

$$
F_1(\mathbf{r}, \mathbf{v}, t) f_1(y, t) = 0. \quad (34)
$$

Proof

T-1) Second, thanks the Lemma [see Eq. (29)], it follows that Eq. (31) of Corollary 1 delivers in the whole space $\Gamma_1 \times I_{o1}$

$$
L^* f_1^{s(N)}(y, t) = \int_{\Gamma_{1(2)}} d\mathbf{x}_2 L^* f_2^{s(N)}(\mathbf{y}, \mathbf{x}_2, t) \equiv L^* f_1^{s(N)}(y, t),
$$

which, denoting $f_1^{s}(y, t) = L^* f_1^{s(N)}(y, t)$, proves also Eq. (33).

T-2) Third, thanks to the Lemma, Eq. (30) delivers Eq. (34). c.v.d.

As consequence, we conclude that the strong B-G limit function $f_1(y, t)$ does not generally satisfy the limit equation (10) of the BBGKY (or Boltzmann) hierarchy, i.e., in other words the strong B-G limit does not exist for the equations of the BBGKY hierarchy.

It is manifest that this result can also be expressed in the following equivalent form:

**Corollary of THM.3**

In validity of THM.3 it follows that

$$
[L^*, F_1] f_1^{s(N)}(x_1, t) \neq 0. \quad (36)
$$

Namely the operators $L^*$ and $F_1$ do not commute. This means that for $S_N$ when applying the B-G limit operator $L^*$ to the equations of the BBGKY hierarchy the limit equations do not generally recover the Boltzmann hierarchy. Hence, we conclude that - in the case of the hard-sphere system here considered - the Lanford conjecture for the BBGKY hierarchy fails, at least if it is intended in the sense of the strong B-G limit here considered.

5 - CONCLUSIONS

The main conclusion of this paper is that the Boltzmann hierarchy and the Boltzmann equation cannot generally be recovered from the BBGKY hierarchy for the system $(S_N)$ of smooth-hard (and impenetrable) spheres, at least in the sense of the strong B-G limit. The discovery appears striking, especially in view of the previous literature appeared on the subject. A related interesting question which obviously arises, in the light of this conclusion, is that of the interpretation of customary results due to Lanford and followers. As is well-known, being all based on the treatment of the smooth-hard sphere problem in terms of formal time-series solution of the BBGKY, they rely on the interpretation of the B-G limit as a weak* limit. This problem is which is particularly relevant in connection with the issue of (local or global) validity of the Boltzmann kinetic equation for the one-particle limit PSPD will be treated elsewhere [30].

In this paper the validity of the Lanford conjecture [3, 13, 17], with particular reference to the BBGKY hierarchy, has been investigated adopting, for this purpose, a $\Gamma_1$-phase-space microscopic statistical description for
the time-evolution of a system of $N$ smooth-hard spheres ($S_N$). The result has been achieved using the Klimontovich approach to MSD for $S_N$. The approach, which can in principle be extended to higher-order joint probability densities, permits to determine a formal exact solution of their time evolution without recurring to cumbersome time-series representations. This allows, in particular, to construct an explicit integral representation for the one-particle probability density, to be expressed in terms of the initial $\Gamma_N$-phase-space microscopic probability density. The key aspect of the approach here developed is - however - the fact that, since the Klimontovich representation does not involve the adoption of time-series representations for the one-particle probability density usually adopted in the customary BBGKY-approaches, it can be used to determine explicitly the strong B-G limit of the joint probability densities. In this paper, in particular, the behavior of the one-particle PSPD has been investigated.

We have shown that the one-particle limit function $f_1(y,t)$, in the sense of the strong B-G limit, does not generally belong to the functional class of the solutions of the corresponding limit equation \[\text{(10)}.\] To reach the proof suitable assumptions on the behavior of the one-particle and the two-particle joint probability densities - as well as for the corresponding limit functions and related quantities - have been invoked. This includes the hypothesis that the one-particle probability density and its limit function are a suitably smooth and bounded ordinary functions. Similar conclusions are expected to apply for arbitrary $s$-particle limit functions (for $s > 1$).

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APPENDIX - $\Gamma_N$-MSD FOR $S_N$

The following basic result is well-known \[\text{3, 8, 12}]:

**Theorem 1 - $\Gamma_N$-MSD for $S_N$**

Let us assume that for $S_N$ (system of $N$ like smooth-hard spheres) there results:

1) for any finite $N > 0$, the initial microscopic probability density $f_N(x_s(t_o))$ is defined as an ordinary function which is at least differentiable in the whole $6N$-dimensional phase space $\Gamma_N = \Omega^N \times \mathbb{R}^{3N}$;

2) $f_N(x_s(t_o))$ is assumed assumed suitably summable so that for any $s = 1, N - 1$ the initial $s$-particle joint probability densities

\[
f_s^{(N)}(x_1,..x_s,t_o) = \int_{\Gamma_{1(s+1)}} dx_{s+1} f_{s+1}^{(N)}(x_1,..x_{s+1},t_o)
\]

are defined and suitably smooth in the $s$-particle phase-space $\Gamma_s = \Omega^s \times \mathbb{R}^{3s}$.

Then it always possible to define uniquely $f_N(x,t)$ in whole set $\Gamma_N \times I$, where $I \equiv \mathbb{R}$ (global existence domain) such that:

A) $f_N(x,t)$ is an ordinary smooth function in whole set $\Gamma_N \times I$;

B) in any open subset of $I$ not containing collision events $f_N(x(t),t)$ is a continuous and differentiable function of time which is constant on all $\Gamma_N$-phase-space trajectories $x(t) = x(x_o, t - t_o)$, i.e. there results, at arbitrary $t, t_o$ belonging to such a time interval and arbitrary admissible initial state $x_o$ belonging to the subset of $\Gamma_N$ in which no collision event occur,

\[
f_N(x(t),t) = f_N(x_o,t_o)
\]

(integral Liouville equation);

C) at an arbitrary collision time $t_c \in I$, $f_N(x(t),t)$ satisfies one of the following boundary conditions: unary collision:

\[
f_N(x_1(t_c),..x_i(t_c),..x_N(t_c),t_c) = f_N(x_1(t_c),..x_i^{(-)}(t_c),..x_N(t_c),t_c);
\]

binary collisions between particles $i$ and $j$ :

\[
f_N(x_1(t_c),..x_i^{(-)}(t_c),x_j^{(-)}(t_c),..x_N(t_c),t_c) = f_N(x_1(t_c),..x_i^{(+)}(t_c),x_j^{(+)}(t_c),..x_N(t_c),t_c);
\]

D) for each $s = 1, N - 1$ the $s$-particle joint probability density

\[
f_s^{(N)}(x_1,..x_s,t) = \int_{\Gamma_{1(s+1)}} dx_{s+1} f_{s+1}^{(N)}(x_1,..x_{s+1},t)
\]

is uniquely defined for all $t \in \mathbb{R}$ and satisfies the equation of the BBGKY hierarchy for $f_s^{(N)}$;

R) for $s = 2, N - 1$ and in any open subset of $I$ not containing collision events involving only the first $s$ particles of $S_N$,

\[
f_s^{(N)}(x_1(t),..x_s(t),t) = \int_{\Gamma_{1(s+1)}} dx_{s+1} f_{s+1}^{(N)}(x_1(t),..x_s(t),x_{s+1},t)
\]
is a continuous and differentiable function of time. (Proof omitted).

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