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BBGKY Hierarchy for Hard Sphere Systems

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Abstract

In the first part of this work, the series expansion for the evolution of the correlation functions of a finite system of hard spheres is derived from direct integration of the solution of the Liouville equation, with minimal regularity assumptions on the density of the initial measure. The usual BBGKY hierarchy of equations is then recovered. A graphical language based on the notion of collision history originally introduced by Spohn is developed, as a useful tool for the description of the expansion and of the elimination of degrees of freedom.

In the second part of the thesis, an integration method is established to construct the Maxwellian solutions to the stationary BBGKY hierarchy of an infinite system of particles, in the case of a smooth, positive and short range potential. A problem of existence and uniqueness of such solutions with appropriate boundary conditions is thus solved. The result is extended in a milder sense to the hard core systems.

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Contents

Chapter 1

Introduction

The BBGKY hierarchy is the fundamental system of equations for the evolution of correlation functions of a state in Classical Statistical Mechanics, [5]. Their 70 years old history has brought enormous progress in the investigation of the transition from the microscopic to the macroscopic world, and they are still an attractive starting point for new developments. In particular, great advance has come by clever methods of truncation, approximation and scaling limits of the hierarchy, providing in various cases a justification of the kinetic equations describing particle systems on mesoscopic (intermediate) scales. The mathematical rigorous achievement of many concerned results is still unsolved. Besides this, the complex mathematical structure of the hierarchy makes it impossible to use the system of equations in its entirety: for this it seems necessary to develop new techniques.

In this thesis I address some problems related to: a) the derivation of the hierarchy from first principles; b) the solution of the complete hierarchy in simple cases. Hopefully, the new results discussed in this work provide a first basic step in a much harder program, that is the use of the BBGKY for the description of systems out of equilibrium.

Over recent years there has been renewed interest on non–equilibrium properties of hard sphere systems, for which the evolution equations, as well as the stationary non–equilibrium equations, are in many respects the easiest possible to treat. This is the reason why this thesis devotes special attention to the systems with such potential. On the other hand, the properties of the hard core dynamics are quite delicate because of the singular character of the interaction. For instance, the analysis of these systems leads naturally to the issue of giving a precise meaning to the BBGKY equations for non regular initial measures: as we will see, in this case a fair description of the evolution of correlation functions is given by a series expansion in the time–zero correlations (the famous one used to derive the Boltzmann equation). Moreover, we will point out in the last chapter that, for purely hard core systems, even the problem of equilibrium solutions of the hierarchy has not been fully investigated.

The thesis is divided into two independent parts, which I introduce respectively in the following two sections. Chapters 2–6 deal with the derivation of the hierarchy for the finite system of hard spheres, while Chapters 7–8 deal mainly with the problem of the integration of the hierarchy for an infinite system with smooth and short range interaction.

1.1 Results and methods I. Derivation

In his famous derivation of the Boltzmann equation [27], O. E. Lanford makes use of a series expansion for the time–evolved correlation functions of a classical finite system of hard spheres in a box. This expresses the $n-$points correlation function at time t as a sum of integral terms involving all the higher order correlation functions at time zero. The expansion is derived, though not rigorously, from iteration of the BBGKY hierarchy of integro–differential equations, and is considered as a "series solution" of its Cauchy problem. A rigorous validation of the hierarchy and of the series has been given years later by H. Spohn in an unpublished note [45], and by R. Illner and M. Pulvirenti in [23] (see also the book [7]), using different methods.

In both the previous papers an assumption on the initial measure is made to derive the BBGKY hierarchy, that is the continuity along trajectories of the hard spheres flow. However, there is no physical reason to expect such a regularity property to hold, and it is worthwhile to notice that the final series expansion makes perfectly sense without assuming it. In fact, Spohn observes at the end of his note, by a density argument, that the expansion can be extended to a more general class of measures having no continuity properties. On the other hand, the interpretation of the BBGKY hierarchy as a family of partial differential equations is not at all easy, nor standard in any case, since it relies on the nontrivial properties of the operator T_t of the hard sphere dynamics. Hence, the series solution concept appears to be more appropriate for the description of the dynamics in terms of probability distributions, and one wonders whether it is possible to derive it without going through the usual hierarchy. The present thesis (Chapters 2–6) is devoted to a derivation of the series expansion for the correlation functions, which is *not* based on the iteration of the BBGKY equations, and never requires continuity along trajectories. We rather construct a method of direct integration of the solution of the Liouville equation, that allows to establish the validity of the expansion in a sense even *stronger* than those obtained in the existing literature: the result holds for all times in a fixed full measure invariant subset of the phase space, exactly as it happens for the existence of the dynamics of the underlying system of particles. The hierarchy of integro–differential equations is then recovered by resummation of the series, *without* additional assumptions on the initial measure, thus strengthening an analogous result in [23].

Let us recall the derivation of Lanford and state our main result in an informal way. Consider the vector of correlation functions $\underline{\rho} = \{\rho_n\}_{n\geq 1}$, where ρ_n is defined over the phase space of n hard spheres of mass m and diameter $a > 0$ in a box Λ. A point in this space is an $n-$tuple $(x_1, \cdots, x_n), x_j = (q_j, p_j)$, specifying position and momentum of the n particles. If N is the total number of particles, we set $\rho_n = 0$ for $n > N$. Then the BBGKY hierarchy for the evolution of ρ can be written

$$\frac{\partial}{\partial t}\underline{\rho}(t) = H\underline{\rho}(t) + Q\underline{\rho}(t) \ , \tag{1.1}$$

where

$$\Big(H\underline{\rho}\Big)_n (x_1, \cdots, x_n, t) \equiv \Big\{H_n, \rho_n\Big\}(x_1, \cdots, x_n, t) \tag{1.2}$$

is the $n-$particles Liouville operator acting on ρ_n (including the effects of elastic collisions) and the collision operator is defined by

$$\Big(Q\underline{\rho}\Big)_n (x_1, \cdots, x_n, t) = a^2 \sum_{j=1}^{n} \int d\hat{p} d\hat{w} \hat{w} \cdot \left(\frac{\hat{p} - p_j}{m}\right) \rho_{n+1}(x_1, \cdots, x_n, q_j + a\hat{w}, \hat{p}, t) \ . \tag{1.3}$$

Here $\hat{p}$ is integrated over all $\mathbb{R}^3$, and $\hat{w}$ runs over the unit sphere.

If $t \longrightarrow T_t(x_1, \cdots, x_n)$ is the flow of the dynamics, define the translation along trajectories of a vector of functions $\underline{f} = \{f_n\}_{n\geq 1}$ as

$$\Big(S(t)\underline{f}\Big)_n (x_1, \cdots, x_n) = f_n(T_{-t}(x_1, \cdots, x_n)) \ . \tag{1.4}$$

Then, integration and iteration of Equation (1.1) leads to the formal solution

$$\underline{\rho}(t) = S(t)\underline{\rho}(0) + \sum_{m=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{m-1}} dt_m S(t-t_1) Q S(t_1-t_2) \cdots Q S(t_m) \underline{\rho}(0) \ . \tag{1.5}$$

In this thesis *we analyze in detail the structure of Eq. (1.5) and prove that it holds, for all times in a full measure subset of the phase space, for any absolutely continuous measure with density symmetric in the particle labels, and bounded by an equilibrium–like distribution. The hierarchy (1.1) can be obtained then, in a mild sense, by taking the derivative,* [44]. No assumption of continuity is needed even for this last operation. We also allow the total number of particles N to be non fixed by the initial measure. The boundedness requirement is stronger than the necessary, and it is the same used by Lanford to control the convergence of the series in the Boltzmann–Grad limit. Here it is made to control easily through all the steps the integrals over momenta of the type (1.3), (1.5).

The main interest of the discussion is the method of the proof. For $n = N$ Eq. (1.5) reduces to the evolution of the density function, that is the solution of the Liouville equation:

$$\rho_N(x_1, \cdots, x_N, t) = \rho_N(T_{-t}(x_1, \cdots, x_N), 0) \ . \tag{1.6}$$

It is desirable that we can construct the series expansion for the ρ_n from *direct integration* of (1.6) over all the phase space of $N - n$ particles compatible with a fixed state $(x_1, \cdots, x_n)$. We show that in fact this can be done by eliminating the degrees of freedom one by one. To achieve the integration of the single degree of freedom, it is important to understand the structure of the right hand side in (1.5). This has been widely studied since the work of Lanford [27], see for instance [24] or [46]. It results that the integrand function in the generic term of the formula, depends on the states assumed by certain clusters of particles following a fictitious evolution: this is constructed from the state $(x_1, \cdots, x_n)$ at time t, by suitably adding more and more particles as the time flows backwards. Following [46], we shall call *collision history* such an evolution.

The collision histories can be represented graphically in terms of special binary tree graphs. Therefore, a graphical picture of the series expansion (1.5) is obtained. This representation is our basic tool. In fact, it turns out that the integration of a degree of freedom itself can be translated in graphical language, through appropriate *operations over tree graphs.* The graphical rules corresponding to the elimination of a single degree of freedom, clarify how the various terms of the expansion for ρ_n emerge from those for ρ_{n+1}, thus considerably simplifying the presentation of the proof. The analytical operations corresponding to these rules, are nothing but a suitable partitioning of the integration domain, and convenient representation (change of variables) of the subsets of the partition. Nevertheless, in order to establish the graphical rules, it is also essential to prove that some classes of collision histories give a net null contribution to the integration of the degree of freedom: this is done again with the help of the tree graphs, by showing explicit one by one *cancellations* among the collision histories of these classes.

The proof will be discussed in Chapter 5, while preliminaries and presentation of results will be respectively the object of Chapters 2–3 and 4.

1.2 Results and methods II. Integration

The understanding of the complete system of BBGKY equations without the use of approximations is an open challenge for physicists and mathematicians. It is often stated that the problem of *solving* the Liouville equation is as difficult as finding the solution to the corresponding full dynamics of particles. Clearly the same is true for the BBGKY hierarchy as soon as the number of particles (hence the system of equations) is *finite*. Nevertheless, if we are concerned with equilibrium or stationary non–equilibrium for thermodynamic systems, we rather deal with an *infinite* set of coupled equations. Hopefully in this case, if the states considered are smooth enough, we *can* deduce non trivial informations from the complete hierarchy of equations. At least, this is what happens in the equilibrium setting, as we shall prove in the present thesis (Chapters 7–8).

Our main aim is to establish a constructive integration method of the stationary hierarchy with boundary conditions. The simplest case to face (in three dimensions) is the thermodynamic *equilibrium hierarchy*, which is the infinite system of equations relating the positional correlation functions, when the momenta have a Maxwellian distribution, and cluster properties of the correlations at infinity are assumed as boundary conditions, together with translation invariance. For this problem (main result of the second part of the thesis, [18]) *we shall carry out an iterative integration leading from the BBGKY to the Kirkwood–Salsburg equations*, a set of integral relations which is well known to be one of the equivalent characterizations of an equilibrium state. This will be done for smooth and short range positive potentials.

The first to notice this equivalence was Morrey in the remarkable paper [33]. There, a lengthy and involved proof did not led from the hierarchy to the Kirkwood–Salsburg equations, but to a complicated expansion which can be proved to be equivalent for small densities. Then Gallavotti e Verboven attempted to give a clear proof of Morrey's theorem in [17], in the same assumptions of small density, strong cluster properties, rotational and translational symmetry. This remained as the only example of a simple method of direct integration of the infinite system. The iterative procedure is carried out for smooth interactions; it is convergent for small densities, and it allows an exponential bound of the error term, which is not uniform in the hard core approximation. Moreover, while looking for a way to extend the procedure to the hard core case, Genovese and the writer found a bug in the proof, which gives an incorrect expression for the activity. The correction, as we will see, makes the procedure slightly involved.

We will present a new simple iterative method providing the outcome with a much faster rate of convergence than that of the previous work: that is factorial against exponential. This allows to extend the result to not necessarily small densities, weak cluster properties and states with simple translation invariance at infinity. Together with the above stated equivalence with the KS equations, the method gives uniqueness of the solution in the small density – high temperature region (resorted to the uniqueness of the solution of the Kirkwood–Salsburg equations). Furthermore, since the radius of convergence of the procedure is uniformly bounded in the hard core limit, it allows to describe the hard core stationary Maxwellian hierarchy as a limit of smooth versions of it: hence to set the uniqueness of its solution within the functions that can be approximated with solutions of the smooth hierarchy, with few restrictions on the form of the approximants.

1.3 Summary

The thesis is organized as follows. In Chapter 2 we define a model of hard spheres, we introduce our notations, state our assumptions on the initial measure and recall the heuristic derivation of the hard spheres BBGKY. In Chapter 3 we introduce the concept of collision history, as well as the graphical rules for its representation, and explain how to represent formula (1.5) in terms of the tree graphs. In Chapter 4 we present the first part of our main results, while in Chapter 5 we discuss the proof of the related main theorem, establishing the above mentioned graphical integration rules, and applying them to the generic inductive step. In Chapter 6 we present the conclusions of the previous discussion and make some comparison with existing literature. In Chapter 7 we introduce the infinite system of particles, state our results on the integration of the corresponding stationary hierarchy, and discuss two different methods for the proof. Finally, in Chapter 8 we make some comments on the solution of the hard core equilibrium hierarchy. Some technical aspects of the proofs are deferred to the Appendices.

Chapter 2

The hard sphere system

In this chapter we set model and notations, which we inherit essentially from [45], and state some preliminary result on the hard sphere dynamics (Section 2.1). In Section 2.2 we introduce the class of measures we will work with, and in Section 2.3 we present the classical heuristic derivation of the BBGKY for hard spheres.

2.1 Model and notations

Let us consider a system of N hard spheres of equal mass m and of diameter $a > 0$ in a box $\Lambda \subset \mathbb{R}^3$. Denote $x_i = (q_i, p_i) \in \Lambda \times \mathbb{R}^3$ the configuration of the i–th particle, $i = 1, \cdots, N$. Λ is bounded and has a piecewise smooth elastically reflecting boundary $\partial\Lambda$.

Between collisions each particle moves on a straight line maintaining unchanged its velocity. In a collision of two hard spheres at positions q_i, q_j with

$$\hat{\omega} = (q_i - q_j)/|q_i - q_j| = (q_i - q_j)/a \in S^2$$

and with *incoming* momenta p'_i, p'_j (that means $(p'_i - p'_j) \cdot \hat{\omega} < 0$), the *outgoing* momenta p_i, p_j (with $(p_i - p_j) \cdot \hat{\omega} > 0$) are given by

$$\begin{aligned} p'_i &= p_i - \hat{\omega}[\hat{\omega} \cdot (p_i - p_j)] \ , \\ p'_j &= p_j + \hat{\omega}[\hat{\omega} \cdot (p_i - p_j)] \ , \end{aligned} \tag{2.1}$$

as a consequence of conservation of momentum and energy. Moreover, in a collision of a particle with momentum p'_i with $\partial\Lambda$ at a regular point q (there is only one point of contact between the wall and the sphere) the reflected outgoing momentum p_i is given by

$$p_i = p'_i - 2\hat{n}(q)(\hat{n}(q) \cdot p'_i) \ , \tag{2.2}$$

where $\hat{n}(q)$ is the inner unit vector normal at q to $\partial\Lambda$. It is easy to see that the collision transformations (2.1) and (2.2) preserve Lebesgue measure on $\mathbb{R}^3 \times \mathbb{R}^3$ and $\mathbb{R}^3$ respectively.

We may introduce the $n-$particle phase space, $n = 1, \cdots, N$,

$$\Gamma_n = \{(x_1, \cdots, x_n) \in (\Lambda \times \mathbb{R}^3)^n \mid |q_i - q| \geq a/2 \text{ for every } q \in \partial\Lambda,\ |q_i - q_j| \geq a,\ i,j = 1, \cdots, n,\ i \neq j\}\ . \tag{2.3}$$

A state of the system is given by a point in the whole phase space Γ_N.

Under few simple regularity assumptions on $\partial\Lambda$ (see [3] for the details) the dynamics determined by (2.1), (2.2) and the free flow has been shown to exist in [3], [32]. More precisely, it has been shown that there exists a subset $\Gamma_n^* \subset \Gamma_n$ of full Lebesgue measure $dx_1 \cdots dx_n$ such that for all $t \in \mathbb{R}$ and for every point $(x_1, \cdots, x_n) \in \Gamma_n^*$ the flow of the $n-$particle dynamics

$$t \mapsto T_t^{(n)}(x_1, \cdots, x_n) \in \Gamma_n^* \tag{2.4}$$

is well defined. For all t the mapping $(x_1, \cdots, x_n) \longrightarrow T_t^{(n)}(x_1, \cdots, x_n)$ is uniquely defined as an invertible transformation from Γ_n^* to Γ_n^*. Moreover, Lebesgue measure on Γ_n^* is preserved by the flow, being preserved at each single collision transformation of the type (2.1), (2.2) The flow can be extended to be a measure preserving map over the whole Γ_n: we refer to [47] for a detailed discussion on the measurability properties.

The set $\Gamma_n \setminus \Gamma_n^*$, which is of null Lebesgue measure, can be defined as the subset of all the points of Γ_n which evolved in time run into either (see for instance [3], page 16):

- a “multiple” collision, that is simultaneous contact of more than two hard spheres or simultaneous contact of two hard spheres with each other and at the same time with $\partial\Lambda$;
- a grazing collision with the wall ($\hat{n}(q) \cdot p_i' = 0$) or a grazing two–body collision ($(p_i' - p_j') \cdot \hat{\omega} = 0$);
- a collision of a particle with a “singular” point of $\partial\Lambda$;
- infinitely many collisions in finite time.

The flow through such situations is not determined. We shall refer to them as the “singular configurations”. Some examples in which a particle undergoes infinitely many collisions in a finite time are given in [3].

Let us mention here a fact related to the properties of the flow. Call Υ the subset of $\partial\Gamma_n$ collecting all the multiple collisions, the simultaneous collisions (more than one collision occurring at the same time), the grazing collisions (between particles or with the walls) and the collisions with non regular points of $\partial\Lambda$. Consider the collision surfaces

$$\begin{aligned}
&\Phi_n^+ = \cup_{i\neq j}\Phi_{n,ij}^+ \;, \\
&\Phi_{n,ij}^+ = \{(x_1,\cdots,x_n)\in\partial\Gamma_n\setminus\Upsilon \text{ s. t. } |q_i-q_j|=a \\
&\qquad\qquad \text{and } q_j = q_i + aw, (p_j-p_i)\cdot w > 0\} \;, \\
&\Phi_{n,ij}^+ = \{(x_1,\cdots,x_n)\in\partial\Gamma_n\setminus\Upsilon \text{ s. t. } |q_i-q_j|=a \\
&\qquad\qquad \text{and } q_j = q_i + aw, (p_j-p_i)\cdot w > 0\} \;,
\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}
&\Psi_n^{+(-)} = \cup_i \Psi_{n,i}^{+(-)} \;, \\
&\Psi_{n,i}^{+(-)} = \{(x_1,\cdots,x_n)\in\partial\Gamma_n\setminus\Upsilon \text{ s. t. } |q_i-q| = a/2 \\
&\text{for some regular } q\in\partial\Lambda, \text{ and } p_i\cdot\hat n(q) > (<)0\} \;.
\end{aligned} \tag{2.6}$$

We have a decomposition of the boundary

$$\partial\Gamma_n = \Phi_n^+ \cup \Phi_n^- \cup \Psi_n^+ \cup \Psi_n^- \cup \Upsilon \;. \tag{2.7}$$

The Lebesgue measure on Γ_n induces, through the flow, a measure $d\sigma_n$ on $\partial\Gamma_n$ ([32], [7]), whose restrictions onto $\Phi_{n,ij}^\pm, \Phi_{n,i}^\pm$ are given respectively by

$$\begin{aligned}
&d\sigma_{n,ij}^\pm = \pm dx_1\cdots dx_i\cdots dx_{j-1}dx_{j+1}\cdots dx_n dp_j dw a^2 w\cdot(p_j-p_i) \;, \\
&d\sigma_{n,i}^\pm = \pm dx_1\cdots dx_{i-1}dx_{i+1}\cdots dx_n dq dp_i p_i\cdot\hat n(q) \;,
\end{aligned} \tag{2.8}$$

where w is the unit vector pointing from q_i to q_j, $\partial\Lambda \ni q, q_i = q+\hat n(q)$, and dq is the measure over the surface $\partial\Lambda$. The set Υ has null σ measure, and the Lebesgue measure on Γ_n can be written as $d\sigma_n dt$, t being the time of the last collision in $\partial\Gamma_n$. In references [32] and [7] it is proved that the flow (2.4) is well defined on $\partial\Gamma_n$, again almost everywhere, with respect to the measure $d\sigma$. This existence property of the hard sphere dynamics is important for the derivation of the BBGKY hierarchy of integro–differential equations, as we will discuss in Section 4.1 (see also [7]).

We shall collect the above results, for easy recall in the future, in the following

Proposition 2.1.1 *(Existence of the dynamics) The set $\Gamma_n\setminus\Gamma_n^*\subset\Gamma_n$ defined by the above list is a null Lebesgue measure subset. Moreover, its intersection with the boundary $\partial\Gamma_n$ is a null measure subset of $\partial\Gamma_n$ with respect to the measure $d\sigma_n$.*

For the proof, we refer to [3], Theorem II.B.2, page 19 (see also [32] and [7]).

As in [45], we do *not* identify ingoing and outgoing momenta, but we regard them as corresponding to distinct points in phase space, so that the flow $T_t^{(n)}$ is only piecewise continuous in t. Then, when necessary, we distinguish the limit from the future $(+)$ and the limit from the past $(-)$ writing

$$T_{t\pm}^{(n)}(x_1,\ldots,x_n) = \lim_{\varepsilon\to 0^+} T_{t\pm\varepsilon}^{(n)}(x_1,\ldots,x_n)\ . \tag{2.9}$$

We list some definitions that will be useful in what follows.

$$\begin{aligned}\Gamma_{N-n}(x_1,\cdots,x_n) = \quad & \{(x_{n+1},\cdots,x_N)\in\Gamma_{N-n}\mid |q_i-q_j|\geq a \\ & \text{for } i=1,\ldots,N \text{ and } j=n+1,\cdots,N\}\ ,\end{aligned} \tag{2.10}$$

for $(x_1,\cdots,x_n)\in\Gamma_n$; that is $\Gamma_{N-n}(x_1,\cdots,x_n)$ is the set of the possible configurations of $N-n$ particles when we have n other particles in $(x_1,\cdots,x_n)$. We call $\Omega_i(x_1,\cdots,x_n,\hat p)$ the points $\hat w$ on the unit sphere surface such that the configuration $(x_1,\cdots,x_n,q_i+a\hat w,\hat p)$ is compatible with the hard core exclusion and it does not run into a singular configuration at any time:

$$\Omega_i(x_1,\cdots,x_n,\hat p) = \{\hat w\in S^2 \mid (x_1,\cdots,x_n,q_i+a\hat w,\hat p)\in\Gamma^*_{n+1}\} \tag{2.11}$$

for $i=1,\ldots,n,\ (x_1,\cdots,x_n)\in\Gamma_n$ and $\hat p\in\mathbb{R}^3$. If

$$\overline{\Omega}_i(x_1,\cdots,x_n) = \{\hat w\in S^2 \mid (x_1,\cdots,x_n,q_i+a\hat w,\hat p)\in\Gamma_{n+1}\ \forall\hat p\in\mathbb{R}^3\}\ , \tag{2.12}$$

then $\overline{\Omega}_i(x_1,\cdots,x_n)\setminus\Omega_i(x_1,\cdots,x_n)$ is a set of null Lebesgue–induced measure on S^2 for almost all $(x_1,\cdots,x_n,\hat p)\in\Gamma_n\times\mathbb{R}^3$, by Proposition 2.1.1. Furthermore we define $\Omega_{i+}(x_1,\cdots,x_n,\hat p)$ ($\Omega_{i-}(x_1,\cdots,x_n,\hat p)$) the points of $\Omega_i(x_1,\cdots,x_n,\hat p)$ corresponding to outgoing (incoming) collisions:

$$\begin{aligned}\Omega_{i+}(x_1,\cdots,x_n,\hat p) &= \{\hat w\in\Omega_i(x_1,\cdots,x_n,\hat p))\mid \hat w\cdot(\hat p-p_i)>0\}\ , \\ \Omega_{i-}(x_1,\cdots,x_n,\hat p) &= \{\hat w\in\Omega_i(x_1,\cdots,x_n,\hat p))\mid \hat w\cdot(\hat p-p_i)<0\}\ ,\end{aligned} \tag{2.13}$$

and analogous definitions for $\overline{\Omega}_{i+}(x_1,\cdots,x_n),\overline{\Omega}_{i-}(x_1,\cdots,x_n)$.

The following subsets of Γ^*_n will be used to describe the time evolution of correlation functions:

$$
\begin{aligned}
&\Gamma_N^{\dagger(0)} = \Gamma_N^{\dagger} = \mathcal{K}_N = \hat{\Gamma}_N = \Gamma_N^* \quad \text{and, for } n < N : \\
&\Gamma_n^{\dagger(0)} = \{\underline{x}_n \in \Gamma_n^* \mid \text{for any } 1 \le k \le N-n, \text{ it is } \underline{x}_{n+k} \in \Gamma_{n+k}^* \\
&\qquad\qquad \text{for almost all } (x_{n+1}, \cdots, x_{n+k}) \in \Gamma_k(\underline{x}_n)\} \ , \\
&\Gamma_n^{\dagger} = \{\underline{x}_n \in \Gamma_n^* \mid \text{for any } 1 \le k \le N-n \text{ and } s \in \mathbb{R}, \\
&\qquad\qquad \text{it is } (T_s^{(n)}(\underline{x}_n), x_{n+1}, \cdots, x_{n+k}) \in \Gamma_{n+k}^* \\
&\qquad\qquad \text{for almost all } (x_{n+1}, \cdots, x_{n+k}) \in \Gamma_k(T_s^{(n)}(\underline{x}_n))\} \\
&\quad \equiv \bigcap_{s \in \mathbb{R}} T_s^{(n)}(\Gamma_n^{\dagger(0)}) \ , \\
&\mathcal{K}_n = \{\underline{x}_n \in \Gamma_n^* \text{ s.t. } (T_s^{(n)}(\underline{x}_n), q_j(s) + a\hat{w}, \hat{p}) \in \mathcal{K}_{n+1} \text{ for all } j = 1, \cdots, n \\
&\qquad\qquad \text{and almost all } (s, \hat{p}, \hat{w}) \in \mathbb{R} \times \mathbb{R}^3 \times \overline{\Omega}_j(T_s^{(n)}(\underline{x}_n)).\} \ , \\
&\hat{\Gamma}_n = \Gamma_n^{\dagger} \bigcap \mathcal{K}_n \ .
\end{aligned}
\tag{2.14}
$$

In the definition of $\mathcal{K}_n$ we put $q_j(s) = (T_s^{(n)}(\underline{x}_n))_{q_j}$. The first two definitions ensure also that $(T_s^{(n)}(\underline{x}_n), x_{n+1}, \cdots, x_{n+k}) \in \Gamma_{n+k}^{\dagger}$ for every k, s and almost all $(x_{n+1}, \cdots, x_{n+k}) \in \Gamma_k(T_s^{(n)}(\underline{x}_n))$. Though it is not clear whether the two sets $\Gamma_n^{\dagger}$ and Γ_n^* coincide for $n < N$, we shall prove, as an extension of the result in Proposition 2.1.1 on the existence of the dynamics, that

$$
\left|\Gamma_n \setminus \Gamma_n^{\dagger}\right| = 0 \ , \tag{2.15}
$$

where $|\cdot|$ denotes Lebesgue measure: see Appendix A, where it is proved also that the restriction of the same set to $\partial\Gamma_n$ is $d\sigma-$null, and that it is

$$
|\Gamma_n \setminus \mathcal{K}_n| = 0 \ . \tag{2.16}
$$

From now on time t is *always supposed to be positive*, without loss of generality. We will use the short notation $\underline{x}_n = x_1, \cdots, x_n$ and, when there is no risk of confusion, and we will simply call "particle i" a particle whose configuration is labelled by an index i. We shall set $m = 1$, since the role of the mass is trivial in all the discussion – see formulas (1.3), (1.5).

2.2 Measures over the phase space

Since all the particles of the system are identical, we will work with the space $\mathcal{L}_N$ of measurable functions $f_N : \Gamma_N \to \mathbb{R}$, symmetric in the particle labels

($f_N(\Pi(x_1,\dots,x_N)) = f_N(x_1,\dots,x_N)$ for any permutation Π), and having a boundedness property of the type

$$|f_N(x_1,\dots,x_N)| \leq A \prod_{j=1}^{N} h_\beta(p_j)\ , \tag{2.17}$$
$$h_\beta(p) = \left(\frac{\beta}{2\pi m}\right)^{\frac{3}{2}} e^{-\frac{\beta}{2m}p^2}$$

on Γ_N, for some $A, \beta > 0$. Suppose to have an initial measure P on Γ_N with density $f_N \in \mathcal{L}_N$ with respect to Lebesgue measure $dx_1 \dots dx_N$,

$$P(dx_1 \dots dx_N) = f_N(x_1,\dots,x_N) dx_1 \dots dx_N\ . \tag{2.18}$$

Then, because the flow $T_t^{(N)}$ preserves the Lebesgue measure, the evolved measure at time t has a density $f_N(t)$ given by

$$f_N(x_1,\dots,x_N,t) = f_N(T_{-t+}^{(N)}(x_1,\dots,x_N)) \tag{2.19}$$

almost everywhere in Γ_N, which is the Liouville equation in a mild form (the $+$ sign is a convention). Points of $\Gamma_N \setminus \Gamma_N^*$ are removed from (2.19). Estimate (2.17) is preserved by the flow by conservation of energy. Hence, $f_N(t) \in \mathcal{L}_N$. Of course since the flow $T_t^{(N)}$ is only defined almost surely, even densities that are regular at time zero will only be $\mathcal{L}_N-$functions at time t.

We define the *correlation functions* $\rho_n, n = 1, 2, \dots$ by

$$\begin{aligned} &\rho_n(x_1,\dots,x_n,t) = N \dots (N-n+1) \cdot \\ &\quad \int_{\Gamma_{N-n}(x_1,\dots,x_n)} dx_{n+1} \dots dx_N f_N(x_1,\dots,x_N,t)\ , \qquad n \leq N\ , \\ &\rho_n = 0\ , \qquad\qquad n > N\ , \\ &\rho_n(x_1,\dots,x_n) \equiv \rho_n(x_1,\dots,x_n,0)\ , \end{aligned} \tag{2.20}$$

where equality is in the space $\mathcal{L}_n$, and points of $\Gamma_n \setminus \Gamma_n^{\dagger(0)}$ are excluded. Observe that

$$|\rho_n(x_1,\dots,x_n,t)| \leq A' \prod_{j=1}^{n} h_\beta(p_j)\ , \tag{2.21}$$

where A' can be taken equal to a pure constant times $N^n|\Lambda|^{N-n}$. The volume of the system $|\Lambda|$ and the diameter of the spheres a will be kept fixed along the whole thesis, and of course by the hard core exclusion N will be bounded by $3|\Lambda|/4\pi a^3$.

Let us say once and for all that, as in the following chapters we work with densities of measures, all equalities will hold for any fixed version of $f_N, f_N(t)$ and $\rho_n(t)$ in their equivalence class, and all statements will be true only almost everywhere in Γ_N or in its subspaces Γ_n. Of course, the subsets where the involved flows of the dynamics are not defined for any time *must be always excluded.* In particular we will show that, assuming (2.19) and (2.20) to be valid over the full measure subsets $\hat{\Gamma}_n$, all derived formulas (and in particular the final expansion) are still valid in the same set. If we like things to be more definite we can always think to fix a version of $f_N, f_N(t)$ assigning, for instance, zero value on the null set $\Gamma_n \setminus \hat{\Gamma}_n$.

We remark that P can be, in general, any measure with density in $\mathcal{L}_n$. In the case P is a probability measure, the quantity

$$\frac{1}{N \cdots (N-n+1)} \int_{\mathcal{W}} dx_1 \cdots dx_n \rho_n(x_1, \cdots, x_n, t) \tag{2.22}$$

is the probability of finding particles $1, 2, \cdots, n$ at time t in the Borel set $\mathcal{W} \in \Gamma_n$.

2.3 Cercignani's derivation of the hierarchy

The idea of constructing the BBGKY integro–differential hierarchy for a system of elastic balls starting from the Liouville equation goes back to papers of Grad in [20]. The first complete deduction was carried out by Cercignani in [6]. This is perhaps the most straightforward derivation, though not mathematically rigorous. In particular, the density $f_N(t)$ is assumed to be *smooth* at all times, so that all the steps to be performed are justified (see the comment after (2.19)). We dedicate the present section to review this derivation. We will use the notations introduced in the previous sections, unless where explicitly specified.

The starting point is the Liouville Equation in its differential form, that is, given a probability density $f_N = f_N(x_1, \cdots, x_N)$ on Γ_N,

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} p_i \cdot \frac{\partial f_N}{\partial q_i} = 0, \qquad (\underline{x}_N \in \Gamma_N^0) \ , \tag{2.23}$$

where Γ_N^0 indicates the interior of Γ_N and $x_i = (q_i, p_i)$. This is simply the usual form of the equation valid for smooth interactions and smooth densities in the region where the state of particles corresponds to inertial motion, so that the term $\sum_{i=1}^N \frac{dp_i}{dt} \cdot \frac{\partial f_N}{\partial p_i}$ drops. Now we want to integrate this equation over its domain of validity, with respect to coordinates and momenta of $N-n$ particles; by symmetry, without loss of generality, we shall integrate with respect to the particles numbered from $n+1$ to N. If we introduce the $n-$particle distribution function defined on Γ_n by formula (2.20), Eq. (2.23) gives:

$$\frac{\partial \rho_n}{\partial t} + N \dots (N-n+1) \sum_{i=1}^{n} \int_{\Gamma_{N-n}(\underline{x}_n)} p_i \cdot \frac{\partial f_N}{\partial q_i} \prod_{l=n+1}^{N} dq_l dp_l \tag{2.24}$$

$$+ N \dots (N-n+1) \sum_{j=n+1}^{N} \int_{\Gamma_{N-n}(\underline{x}_n)} p_j \cdot \frac{\partial f_N}{\partial q_j} \prod_{l=n+1}^{N} dq_l dp_l = 0 \ ,$$

where terms with $1 \leq i \leq n$ have been separated from those with $n+1 \leq i \leq N$ for later convenience.

A typical term in the first sum in Eq. (2.24) contains the integral of a derivative with respect to a variable, q_i, over which one does not integrate; it is not possible, however, to exchange the orders of integration and differentiation because the domain has boundaries ($|q_i - q_l| = a$) depending upon q_i. To obtain the correct result, a boundary term has to be added:

$$\begin{aligned} & N \ldots (N-n+1) \int_{\Gamma_{N-n}(\underline{x}_n)} p_i \cdot \frac{\partial f_N}{\partial q_i} \prod_{l=n+1}^{N} dq_l dp_l \qquad (2.25) \\ &= N \ldots (N-n+1) p_i \cdot \frac{\partial}{\partial q_i} \int_{\Gamma_{N-n}(\underline{x}_n)} f_N \prod_{l=n+1}^{N} dq_l dp_l - N \ldots (N-n+1) \\ &\quad \cdot \sum_{j=n+1}^{N} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3} \left(\int_{\Gamma_{N-n-1}(\underline{x}_n, x_j)} f_N \prod_{\substack{l=n+1 \\ l\neq j}}^{N} dq_l dp_l \right) p_i \cdot \hat{\omega}_{ij} d\sigma_{ij} dp_j \\ &= p_i \cdot \frac{\partial \rho_n}{\partial q_i} - \frac{1}{N-n} \sum_{j=n+1}^{N} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3} \rho_{n+1} p_i \cdot \hat{\omega}_{ij} d\sigma_{ij} dp_j \end{aligned}$$

where $\hat{\omega}_{ij}$ is the outer normal to the sphere $|q_i - q_j| = a$ (with its center at q_j), $d\sigma_{ij}$ the surface element on the same sphere and ρ_{n+1} is the $(n+1)-$particle distribution function with arguments $(q_k, p_k), k = 1, 2, \cdots, n, j$.

A typical term in the second sum in Eq. (2.24) can be immediately integrated by means of the Gauss theorem, since it involves the integration of a derivative taken with respect to one of the variables of integration. We find:

$$\begin{aligned} & N \ldots (N-n+1) \int_{\Gamma_{N-n}(\underline{x}_n)} p_j \cdot \frac{\partial f_N}{\partial q_j} \prod_{l=n+1}^{N} dq_l dp_l \qquad (2.26) \\ &= \frac{1}{N-n} \sum_{i=1}^{n} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3} \rho_{n+1} p_j \cdot \hat{\omega}_{ij} d\sigma_{ij} dp_j + \frac{1}{(N-n)(N-n-1)} \\ &\quad \cdot \sum_{\substack{k=n+1 \\ k\neq j}}^{N} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3\times\Gamma_1(\underline{x}_n)} \rho_{n+2} p_j \cdot \hat{\omega}_{kj} d\sigma_{kj} dp_j dq_k dp_k \\ &\quad + \frac{1}{N-n} \int_{\partial\Lambda} \rho_{n+1} p_j \cdot \hat{n}_j dS_j dp_j \end{aligned}$$

where dS_j is the surface element of the boundary of the region Λ in the three–dimensional subspace described by q_j, and $\hat{n}_j$ is the unit vector normal to such a surface element and pointing into the gas. The last term in Eq. (2.26) is the contribution from the solid boundary of Λ; if the particles are specularly reflected there (see Eq. (2.2)), then the term under consideration is obviously zero because

$p_j \cdot \hat{n}_j$ changes its sign under specular reflection. We shall point out that the boundary term is also zero under more general assumptions: it is sufficient to assume that the effect of an interaction of a rigid sphere with the wall is independent of the evolution of the state of the other spheres and that no particles are captured by the solid walls; see [6], pages 50–52, for more informations.

Inserting Eqs. (2.26) and (2.25) into (2.24), we find:

$$\frac{\partial \rho_n}{\partial t} + \sum_{i=1}^{n} p_i \cdot \frac{\partial \rho_n}{\partial q_i} = \frac{1}{N-n} \sum_{i=1}^{n} \sum_{j=n+1}^{N} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3} \rho_{n+1} V_{ij} \cdot \hat{\omega}_{ij} d\sigma_{ij} dp_j \tag{2.27}$$
$$+\frac{1}{2}\frac{1}{(N-n)(N-n-1)} \sum_{\substack{k,j=n+1\\k\neq j}}^{N} \int_{\overline{\Omega}_j(\underline{x}_n)\times\mathbb{R}^3\times\Gamma_1(\underline{x}_n)} \rho_{n+2} V_{kj} \cdot \hat{\omega}_{kj} d\sigma_{kj} dp_j dq_k dp_k$$

where $V_{ij} = p_i - p_j$ is the relative momentum of the $i-$th particle with respect to the $j-$th and we have taken into account that $p_j \cdot \hat{\omega}_{kj}$ can be replaced by $\frac{1}{2} V_{kj} \cdot \hat{\omega}_{kj}$ in the second sum because of the antisymmetry of $\hat{\omega}_{kj}$ with respect to its own indices. In Eq. (2.27) q_j and p_j are integration variables; hence the sums over j are made up of identical terms, as well as the sums over k in the second integral. We shall write $q_*, p_*, \overline{\Omega}_*$ in place of $q_j, p_j, \overline{\Omega}_j$ in order to emphasize that the index j is dummy, and q_0, p_0 in place of q_k, p_k, while we shall simply write $V_i, \hat{\omega}_i, d\sigma_i$ for $V_{ij}, \hat{\omega}_{ij}, d\sigma_{ij}$ and $V_0, \hat{\omega}_0, d\sigma_0$ for $V_{kj}, \hat{\omega}_{kj}, d\sigma_{kj}$. Accordingly we obtain:

$$\frac{\partial \rho_n}{\partial t} + \sum_{i=1}^{n} p_i \cdot \frac{\partial \rho_n}{\partial q_i} = \sum_{i=1}^{n} \int_{\overline{\Omega}_*(\underline{x}_n)\times\mathbb{R}^3} \rho_{n+1} V_i \cdot \hat{\omega}_i d\sigma_i dp_* \tag{2.28}$$
$$+\frac{1}{2} \int_{\overline{\Omega}_*(\underline{x}_n)\times\mathbb{R}^3\times\Gamma_1(\underline{x}_n)} \rho_{n+2} V_0 \cdot \hat{\omega}_0 d\sigma_0 dp_* dq_0 dp_0$$

where the arguments of ρ_{n+1} are $(q_1, p_1, \cdots, q_n, p_n, q_*, p_*, t)$ and those of ρ_{n+2} are $(q_1, p_1, \cdots, q_n, p_n, q_*, p_*, q_0, p_0, t)$.

Observe that simultaneous contacts of more than two spheres contribute nothing to the above integrals, if ρ_{n+1}, ρ_{n+2} are integrable functions. In fact, such multiple collisions correspond to the contribution to the integrals with respect to $d\sigma_i, d\sigma_0$, coming from the *boundary* of $\overline{\Omega}_*(\underline{x}_n)$ (the last being a surface in $\mathbb{R}^3$), which is a one–dimensional subset. Accordingly, their contribution to the integrals is zero, unless singularities occur, which we *exclude* here by using a smooth f_N.

Now an important remark: *the equations used so far are incomplete, because we have not used the laws of elastic impact, Eq. (2.1).*

According to these laws, in the last formula, any particle entering a collision with momentum p_i' at q_i is at the same time (or a vanishingly short time later) in an after–collision state with momentum p_i related to p_i' and $\hat{\omega}_i$ by

$$\begin{aligned} p_i' &= p_i - \hat{\omega}_i(\hat{\omega}_i \cdot V_i) \\ p_*' &= p_* + \hat{\omega}_i(\hat{\omega}_i \cdot V_i) \ ; \end{aligned} \tag{2.29}$$

this suggests to assume the following:

$$\begin{aligned} &\rho_{n+1}(q_1, p_1, \cdots, q_i, p_i, \cdots, q_n, p_n, q_*, p_*, t) \\ &= \rho_{n+1}(q_1, p_1, \cdots, q_i, p_i - \hat{\omega}_i(\hat{\omega}_i \cdot V_i), \cdots, q_n, p_n, q_*, p_* + \hat{\omega}_i(\hat{\omega}_i \cdot V_i), t) \end{aligned} \tag{2.30}$$

for $i = 1, \cdots, n$ and $1 \leq n \leq N-1$.

Now we examine the term involving ρ_{n+2} in Eq. (2.28) and claim that it is zero, as a consequence of (2.30). First, we separate the integral into the corresponding integrals extended to the subsets $V_0 \cdot \hat{\omega}_0 < 0$ (particles entering a collision) and $V_0 \cdot \hat{\omega}_0 > 0$ (particles that have just collided). The considered term becomes

$$\begin{aligned} &\frac{1}{2} \int_{\overline{\Omega}_{*+}(\underline{x}_n) \times \mathbb{R}^3 \times \Gamma_1(\underline{x}_n)} \rho_{n+2} |V_0 \cdot \hat{\omega}_0| d\sigma_0 dp_* dq_0 dp_0 \\ &\quad - \frac{1}{2} \int_{\overline{\Omega}_{*-}(\underline{x}_n) \times \mathbb{R}^3 \times \Gamma_1(\underline{x}_n)} \rho_{n+2} |V_0 \cdot \hat{\omega}_0| d\sigma_0 dp_* dq_0 dp_0 \ . \end{aligned} \tag{2.31}$$

We may show that the two terms in this formula cancel each other.

In fact, changing the variables from p_0 and p_* to p_0' and p_*' given by Eq. (2.29) with $i = 0$, and taking Eq. (2.30) (with $i = 0$ and n replaced by $n+1$) into account, the *first* term of (2.31) becomes equal to

$$\frac{1}{2} \int_{\overline{\Omega}_{*-}(\underline{x}_n) \times \mathbb{R}^3 \times \Gamma_1(\underline{x}_n)} \rho_{n+2}' |V_0' \cdot \hat{\omega}_0| d\sigma_0 dp_*' dq_0 dp_0' \tag{2.32}$$

where the arguments of ρ_{n+2}' are the same as in ρ_{n+2} with p_* and p_0 replaced by p_*' and p_0', and we have taken into account that the absolute value of the Jacobian determinant of the transformation from p_*, p_0 to p_*', p_0' is 1. The integral extends to the emisphere $V_0' \cdot \hat{\omega}_0 < 0$, because Eq. (2.29) (with $i = 0$) implies

$$V_0 = V_0' - 2\hat{\omega}_0(\hat{\omega}_0 \cdot V_0') \ , \tag{2.33}$$

hence

$$V_0 \cdot \hat{\omega}_0 = -V_0' \cdot \hat{\omega}_0 \ . \tag{2.34}$$

We can now drop the primes in Eq. (2.32), since p_0' and p_*' are integration variables: we find

$$\frac{1}{2} \int_{\overline{\Omega}_{*-}(\underline{x}_n) \times \mathbb{R}^3 \times \Gamma_1(\underline{x}_n)} \rho_{n+2} |V_0 \cdot \hat{\omega}_0| d\sigma_0 dp_* dq_0 dp_0 \ , \tag{2.35}$$

so that the expression in Eq. (2.31) is equal to zero.

Our final result is then

$$\frac{\partial \rho_n}{\partial t} + \sum_{i=1}^{n} p_i \cdot \frac{\partial \rho_n}{\partial q_i} = \sum_{i=1}^{n} \int_{\overline{\Omega}_*(\underline{x}_n)\times\mathbb{R}^3} \rho_{n+1} V_i \cdot \hat{\omega}_i a^2 d\hat{\omega}_i dp_* \qquad (n = 1, \cdots, N) \quad (2.36)$$

for $\underline{x}_n \in \Gamma_n^0$, where we have replaced $d\sigma_i$ by its expression $a^2 d\hat{\omega}_i$ in terms of the radius a of the sphere $|q_* - q_i| = a$ and the element of solid angle $d\hat{\omega}_i$. We shall call this system of equations the BBGKY hierarchy for a hard sphere gas. Its physical meaning is quite transparent: the $n-$particle distribution function evolves in time according to the $n-$particle dynamics, corrected by the effect of the interaction with the remaining $(N - n)$ particles. The effect of this interaction is described by the right hand side of Eq. (2.36).

We stress the fact that the hierarchy (2.36) was derived only under the assumptions of:

- a symmetrical dependence of ρ_n upon the particles;
- a sufficient regularity of ρ_n at all times;
- the validity of condition (2.30)
- assumptions on the boundary $\partial\Lambda$ neglecting the surface integral in the last line of (2.26) (see the comment after (2.26)).

The second item in the list is in particular required in order to neglect the contribution of a *line* to a surface integral, i.e. to neglect the effect of triple collisions.

In [23] the rigorous versions of property (2.30) and of Eq. (2.36) are presented (see also Remark (1) in Chapter 4 of this thesis and Eq. (4.12)). In the following chapters (3 to 6) of the present thesis we will establish a more appropriate rigorous description for the evolution of correlation functions starting from any initial measure with measurable density (plus some decay behaviour for large momenta), and we will derive the BBGKY hierarchy as presented in [23], showing uselessness of condition (2.30).

Chapter 3

Collision histories

In this chapter we analyze the structure of the expansion on the right hand side of (1.5). This is given in general by a large variety of terms. In each of these terms the integrand function contains a time–zero correlation function evaluated in a configuration of particles which can be found by flowing backwards in time the configuration $\underline{x}_n$, and suitably *adding* new particles at the times t_1, t_2 etcetera. The new particles appear in a collision configuration with one of the pre–existent particles. This describes a special (fictitious) evolution that will be called “collision history”, a name first used by Spohn in [45].

In order to have a clear picture of the many terms of the expansion, and of the configurations of particles involved in them, we shall establish rules for their graphical representation. In particular, we will show that Equation (1.5) can be written as a sum over a set of tree graphs. We will introduce the convenient class of trees in Section 3.1: a class of decorated trees to be associated to the collision histories (as explained in Section 3.2), and a class of trees with less decorations corresponding to the terms of the expansion. We will give the rules for this correspondence in Section 3.3, where also an explicit formula will be given for the generic term of the expansion.

We want to stress since the beginning that the collision history is *not* a real trajectory of the particle system, and the associated collisions are *not* a sequence of real collisions. The correspondence between collision histories and sequences of real collisions is only very indirect ([45]).

3.1 A family of trees

We begin by considering binary tree graphs with generic node as in Figure 3.1: one segment *crosses* the node while the other segment is *generated* by the node. In all the diagrams time will always flow from right to left along a horizontal axis. We shall agree to draw the trees in such a way that the root corresponds to time t while the endpoints correspond to time zero, and that one of the two above mentioned segments attached to the node is horizontal, while the other has a (meaningless) slope between 0 and $\pi/2$. We call *line* of a tree the straight segment which left extremum is its generating node (or the root of the tree) and which right extremum is one of the endpoints of the tree.

No trees will be considered with two or more nodes corresponding to the same time. Call

$$\overline{\Delta}(\underline{x}_n; [0,t])$$

for $1 \leq n \leq N, \underline{x}_n \in \Gamma_n^*, t \in \mathbb{R}$, the set of all such binary trees with a number of nodes m variable in $(0, \cdots, N-n)$, exactly $m+1$ lines (and endpoints), and no decoration other than the following:

1. a label $\underline{x}_n$ attached to the root;
2. for $n > 1$, a label $j \in (1, \cdots, n)$ attached to each node crossed by the line ending in the root of the tree.

We avoid to add a label t to the root of the trees if no confusion arises. See Figure 3.2 for an example. We may set $\overline{\Delta}(\underline{x}_n; [0,t]) = \emptyset$ for $n > N$.

We can always think to order the nodes of the tree from left to right with an index $k = 1, 2, \ldots, m$, which we call *ordering number* of the node. We refer to the line generated in the $k-$th node as the *$k-$th line*, and we refer to the line ending in the root of the tree as the *root line*. When the $k-$th node is crossed by the root line we denote j_k the label associated to it.

Two trees will be considered *equivalent* if they can be superposed, together with their labels and without altering their topological structure *neither the ordering of its nodes*. Hence, even though the nodes of a tree are not associated to precise values of the time, they are ordered along the time axis. For given number of nodes m and forgetting about decorations, there will be $m!$ different trees in $\overline{\Delta}(\underline{x}_n; [0,t])$; each of these trees can be decorated with the j labels in n^{m_0} different ways, m_0 being the number of nodes crossed by the root line.

Now take a tree $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t])$. Sometimes we will also use the notation $\overline{\mathcal{D}} = (\underline{x}_n, \overline{\delta})$ to remember that we fixed the root configuration. We shall call *collision history* and indicate it by $\mathcal{D} = (\underline{x}_n, \delta)$, the tree obtained from $\overline{\mathcal{D}}$ by adding a triple $(t_k, \hat{p}_k, \hat{w}_k) \in \mathbb{R} \times \mathbb{R}^3 \times S^2$ to the $k-$th node for every $k = 1, 2, \ldots, m$, where

- t_k is a time variable, so that $t_{m+1} \equiv 0 < t_m < \cdots < t_1 < t_0 \equiv t$;

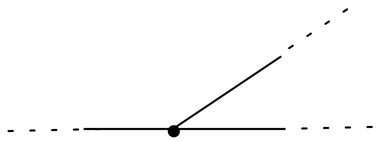

Figure 3.1. Structure of the generic node of a tree: one of the two lines is generated in the node, representing a new particle appearing in the collision histories described by the tree.

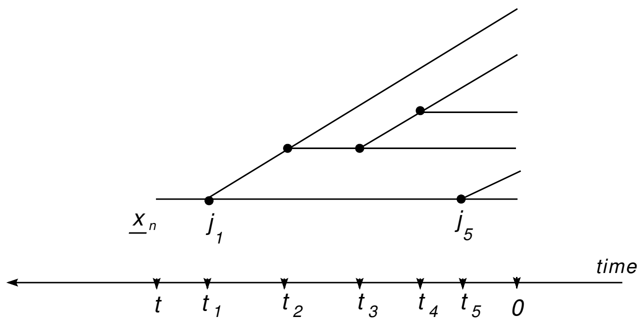

Figure 3.2. Example of tree in $\overline{\Delta}(\underline{x}_n;[0,t])$. It will appear in the expansion for the $n-$points correlation function ($n \leq N-5$); here $j_1, j_5 \in (1,\cdots,n)$. In the figure $0 < t_2 < t_1 < t$.

- $\hat{p}_k$ is a momentum variable;
- the unit vector variable $\hat{\omega}_k$ has some complicated constraint depending on the other labels attached to the tree, which is defined in Section 3.2.

Call also

$$\Delta(\underline{x}_n;[0,t])$$

the space of all the collision histories obtained in this way from $\overline{\Delta}(\underline{x}_n;[0,t])$ for $n \leq N$, and set $\Delta(\underline{x}_n;[0,t]) = \emptyset$ for $n > N$. See Figure 3.3 for some example.

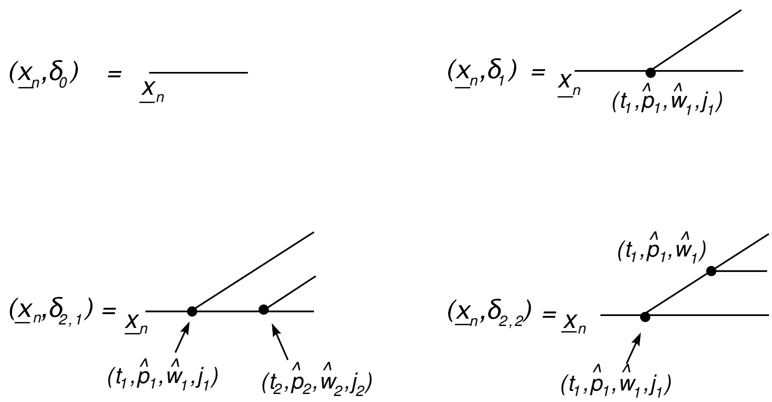

Figure 3.3. Collision histories in $\Delta(\underline{x}_n;[0,t])$ with $0, 1$ or 2 nodes.

Observe that our definition of collision history corresponds to the original one given in [45]. In fact $\Delta(\underline{x}_n;[0,t])$ is in a one by one correspondence with the subset of

$$\bigcup_{0\leq m\leq N-n} (\mathbb{N}\times\mathbb{R}\times\mathbb{R}^3\times S^2)^m \tag{3.1}$$

given by the collections $(m, j_1,\ldots,j_m,t_1,\ldots,t_m,\hat{p}_1,\ldots,\hat{p}_m,\hat{w}_1,\ldots,\hat{w}_m)$ with the above mentioned constraints over times and unit vectors, and with the variables $j_k\in\mathbb{N}$ defined by

$$\begin{aligned} j_k = &\ \text{label attached to the } k\text{−th node,} \\ &\qquad\qquad \text{if the k–th node is crossed by the root line;} \\ j_k = &\ n+q\ , \\ &\qquad\qquad \text{if the k–th node is crossed by the } q\text{−th line}\ , 1\leq q\leq k-1\ . \end{aligned} \tag{3.2}$$

Notice that $1\leq j_k\leq n+k-1$. In the notations $\mathcal{D}=(\underline{x}_n,\delta),\overline{\mathcal{D}}=(\underline{x}_n,\overline{\delta})$, we can identify δ and $\overline{\delta}$ with the corresponding collections of variables:

$$\begin{aligned} \delta &= (m,j_1,\ldots,j_m,t_1,\ldots,t_m,\hat{p}_1,\ldots,\hat{p}_m,\hat{w}_1,\ldots,\hat{w}_m)\ , \\ \overline{\delta} &= (m,j_1,\ldots,j_m)\ . \end{aligned} \tag{3.3}$$

3.2 The fictitious evolution of particles

Let us now construct an evolution of particles

$$\mathcal{E}_{\mathcal{D}}$$

to associate to the history $\mathcal{D}=(\underline{x}_n,\delta)$. The root of a tree is labeled by our starting configuration representing n particles at time t. In general the root line will represent these n particles from time 0 to time t, and the k–th line the $(n+k)$–th particle, $k=1,2,\cdots$, from time 0 to time t_k. The $k-$th node represents a binary collision between the particles associated to the crossed line and the generated line ($(n+k)-$th particle), and the triple $(t_k,\hat{p}_k,\hat{w}_k)$ specifies the time of collision and the momentum and position of particle $(n+k)$ colliding: the vector joining the two particles involved in the collision and pointing towards particle $(n+k)$ will be $a\hat{w}_k$. Finally, the extra label $j_k\in(1,\ldots,n)$ in the nodes crossed by the root line tells us with which particle occurs the collision with particle $(n+k)$.

Given $i=1,2,\cdots,n+m$ ($m=$ number of nodes), we call

$$x_i(s;\mathcal{D})$$

the configuration of the i–th particle at time s in the evolution $\mathcal{E}_{\mathcal{D}}$ (and we will put $x_i(\mathcal{D}) \equiv x_i(0;\mathcal{D})$ for short) and we define this configuration for $0 \leq s \leq t$ by the following construction. Take the root configuration $\underline{x}_n \in \Gamma^*_n$, put $x_i(t;\mathcal{D}) = \underline{x}_n$, and evolve it backwards in time as if there were no other particles in the space up to time t_1 if $m > 0$ (that is with the flow $T^{(n)}_{-t+t_1+}$), and up to time 0 if $m = 0$. This defines $\underline{x}_n(s;\mathcal{D})$ for $t_1 \leq s < t$. At time t_1 stop your ($n-$particle) system and add particle $(n+1)$ in a state $x_{n+1}(t_1;\mathcal{D})$ with momentum $\hat{p}_1$ and position at distance $a\hat{w}_1$ from particle j_1, with $\hat{w}_1 \in \Omega_{j_1}(\underline{x}_n(t_1;\mathcal{D}), \hat{p}_1)$: at fixed $\underline{x}_n, t_1$ we will have either an *incoming* or an *outgoing* collision between particles j_1 and $(n+1)$, depending on the chosen values of $\hat{p}_1, \hat{w}_1$. Then evolve backwards in time particles $(1, \dots, n+1)$ as if there were no other particles in the space up to time $t_2 < t_1$ (with $T^{(n+1)}_{-t_1+t_2+}$); notice that soon after t_1 particle j_1 in the evolution $\mathcal{E}_{\mathcal{D}}$ will deviate from its free motion *if and only* if $\hat{p}_1, \hat{w}_1$ correspond to an *outgoing* collision. At time t_2 stop the system and add particle $(n+2)$ as above with momentum $\hat{p}_2$ and position at distance $a\hat{w}_2$ from particle j_2 (defined by (3.2)), with $\hat{w}_2 \in \Omega_{j_2}(\underline{x}_{n+1}(t_2;\mathcal{D}), \hat{p}_2)$. Later on evolve your $(n+2)-$particle system backwards up to time $t_3 < t_2$, and so on up to the final step, which is the evolution of particles $(1, \dots, n+m)$ with the flow $T^{(n+m)}_{-t_m+}$ from time $t_m > 0$ to time 0. We stress that the configurations $\underline{x}_n(s;\mathcal{D})$ are always constructed by taking limits from the *future*. An example is pictured in Figure 3.4.

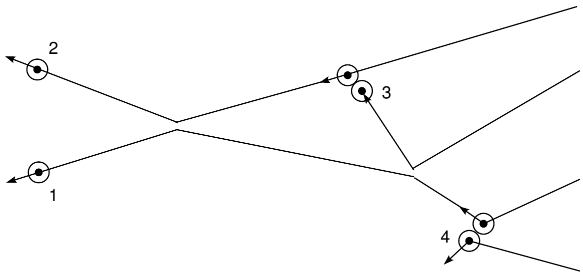

Figure 3.4. Trajectory drawn by the particles in a collision history of the type $(\underline{x}_n, \delta_{2,1})$ of Figure 3.3, in the case $n = 2, j_1 = 2, \hat{w}_1 \in \Omega_{2-}, j_2 = 1, \hat{w}_2 \in \Omega_{1+}$.

In the following we will call

$$\mathcal{E}_{\mathcal{D}}(s)$$

the *configuration* of all the particles of $\mathcal{E}_{\mathcal{D}}$ at time s, without specifying the number of such particles, so that $\mathcal{E}_{\mathcal{D}} = \{\mathcal{E}_{\mathcal{D}}(s)\}_{0\leq s\leq t}$. In particular if s coincides with the time t_k associated to a node, then $\mathcal{E}_{\mathcal{D}}(s)$ is the configuration of the particles of the evolution *after* having added the new particle generated in the node: $\mathcal{E}_{\mathcal{D}}(t_k) = (\underline{x}_{n+k-1}(t_k;\mathcal{D}), q_{j_k}(t_k;\mathcal{D}) + a\hat{w}_k, \hat{p}_k)$. We call

$$N_{\mathcal{D}}(s)$$

the *number of particles* of $\mathcal{E}_\mathcal{D}$ at time s, $N_\mathcal{D}(s) \in (n, \ldots, n+m)$, and we name *cluster of particles* of $\mathcal{E}_\mathcal{D}$ the time–dependent collection of particles described by the evolution.

If we would prefer formulas instead of trees we should write, referring for instance to the trees in Figure 3.3,

$$\begin{aligned}
&\underline{x}_n(s; \underline{x}_n, \delta_0) = T^{(n)}_{-s+}(\underline{x}_n) \ , \quad t \geq s \geq 0 \ , \\
&\underline{x}_n(s; \underline{x}_n, \delta_1) = T^{(n)}_{-s+}(\underline{x}_n) \ , \quad t \geq s \geq -t + t_1 \ , \\
&\underline{x}_{n+1}(\underline{x}_n, \delta_1) = T^{(n+1)}_{-t_1+}(T^{(n)}_{-t+t_1+}(\underline{x}_n), q_{j_1}(t_1; \underline{x}_n, \delta_1) + a\hat{w}_1, \hat{p}_1) \ , \\
&\underline{x}_{n+2}(\underline{x}_n, \delta_{2,1}) = T^{(n+2)}_{-t_2+}\Big(T^{(n+1)}_{-t_1+t_2+}\Big(T^{(n)}_{-t+t_1+}(\underline{x}_n), q_{j_1}(t_1; \underline{x}_n, \delta_{2,1}) + a\hat{w}_1, \hat{p}_1\Big) \ , \\
&\qquad\qquad\qquad\qquad\qquad\qquad q_{j_2}(t_2; \underline{x}_n, \delta_{2,1}) + a\hat{w}_2, \hat{p}_2\Big) \ ,
\end{aligned} \tag{3.4}$$

and so on.

Remarks.

(1) Clearly all this construction is not well defined for $\underline{x}_n \in \Gamma_n \setminus \Gamma^*_n$; definition (2.11) ensures that the added particles do not run the system in a singular configuration.

(2) As we anticipated above, the evolution $\mathcal{E}_\mathcal{D}$ *is not* a real trajectory although it is constructed with pieces of possible real trajectories, and a collision history $\mathcal{D}$ *is not* a sequence of real collisions of the system. In particular, notice that the configuration $x_{n+k}(s; \mathcal{D})$ given by $\mathcal{D}$ is defined only for times $0 \leq s \leq t_k$, and that in general

$$\mathcal{E}_\mathcal{D}(t_k)$$

is different from the limits of $\mathcal{E}_\mathcal{D}(s)$ as $s \to \pm t_k$.

(3) Given the graph $(\underline{x}_n, \delta)$, if particles j_k and $n+k$ are attached to a node with time index t_k, then in $\mathcal{E}_\mathcal{D}$ for times $s \in [0, t_k]$ they can collide many other times between them and with the other particles appearing in the graph at those times, but *not* with other particles of the system that do not appear in the graph. In general any two particles appearing in the graph at a given time can be in a collision configuration.

3.3 Lanford's expansion. A graphical representation

Suppose $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t]), \underline{x}_n \in \Gamma^*_n$, to have m nodes, $m \in (0, \cdots, N-n)$, and order them from left to right with the index $k, 1 \leq k \leq m$ as in Section 3.1. The tree will be associated to collision histories $\mathcal{D} \in \Delta(\underline{x}_n; [0,t])$, obtained attaching to the nodes of $\overline{\mathcal{D}}$ triples $(t_k, \hat{p}_k, \hat{w}_k)$, as explained in the same section, and – see Eq. (3.3) – the two graphs will correspond to collections of variables

$$\begin{aligned} \overline{\mathcal{D}} &= (\underline{x}_n, m, j_1, \cdots, j_m) \ , \\ \mathcal{D} &= (\overline{\mathcal{D}}, t_1, \cdots, t_m, \hat{p}_1, \cdots, \hat{p}_m, \hat{w}_1, \cdots, \hat{w}_m) \ , \end{aligned} \tag{3.5}$$

where $j_1, \cdots, j_m$ are defined via (3.2).

We denote

$$V(\overline{\mathcal{D}})$$

the *value of the tree* $\overline{\mathcal{D}}$ given by the rules summarized in what follows. Going from left to right, *i.e. climbing* the tree:

- associate to the $k-$th node of the tree a *weight factor*

$$W_k(\mathcal{D}) = a^2 \hat{w}_k \cdot (\hat{p}_k - p_{j_k}(t_k; \mathcal{D})) \ ; \tag{3.6}$$

- associate to the $k-$th node of the tree an integration over a subset of $\mathbb{R} \times \mathbb{R}^3 \times S^2$ given by

$$\int_0^{t_{k-1}} dt_k \int_{\mathbb{R}^3} d\hat{p}_k \int_{\Omega_{j_k}(\underline{x}_{n+k-1}(t_k;\mathcal{D}),\hat{p}_k)} d\hat{w}_k \tag{3.7}$$

  (remember that $t \equiv t_0$) where $d\hat{w}_k$ is the natural induced measure on Ω_{j_k};

and at the end

- associate to the $m+1$ endpoints of the tree the $(n+m)-$th correlation function at time zero evaluated in the final configuration of $\mathcal{E}_{\mathcal{D}}$, that is

$$\rho_{n+m}(x_1(\mathcal{D}), \cdots, x_{n+m}(\mathcal{D})) \ . \tag{3.8}$$

Hence $V(\overline{\mathcal{D}})$ can be seen as an integral over times, momenta and unit vector variables attached to the nodes of the collision history $\mathcal{D} \in \Delta(\underline{x}_n; [0,t])$, of a product of a correlation function times a *weight function*

$$W(\mathcal{D}) = \prod_{k=1}^{m} W_k(\mathcal{D}) \ . \tag{3.9}$$

Explicitly,

$$\begin{aligned} V(\overline{\mathcal{D}}) = & \int_0^t dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j_1}(\underline{x}_n(t_1;\mathcal{D}),\hat{p}_1)} d\hat{w}_1 \\ & \cdot \int_0^{t_1} dt_2 \int_{\mathbb{R}^3} d\hat{p}_2 \int_{\Omega_{j_2}(\underline{x}_{n+1}(t_2;\mathcal{D}),\hat{p}_2)} d\hat{w}_2 \dots \\ & \cdot \int_0^{t_{m-1}} dt_m \int_{\mathbb{R}^3} d\hat{p}_m \int_{\Omega_{j_m}(\underline{x}_{n+m-1}(t_m;\mathcal{D}),\hat{p}_m)} d\hat{w}_m R(\mathcal{D}) \ , \end{aligned} \tag{3.10}$$

where R is called *value of a collision history* and is defined by

$$R(\mathcal{D}) = W(\mathcal{D})\rho_{n+m}(x_1(\mathcal{D}), \cdots, x_{n+m}(\mathcal{D})) \tag{3.11}$$

which will be, in our assumptions of Chapter 2, a measurable function over the domain of integration in (3.10) for almost all $\underline{x}_n \in \Gamma_n$. Formula (3.10) is a representation for the generic term of the expansion (1.5). The domain of integration in (3.10) is *maximal* for all times if $\underline{x}_n \in \mathcal{K}_n$, see (2.14). In fact $\mathcal{K}_n$ is defined as the maximal set of values of $\underline{x}_n$ for which the evolutions $\mathcal{E}_{(\underline{x}_n,\delta)}$ (hence their value $R(\underline{x}_n, \delta)$) appearing in the evaluation of $V(\overline{\mathcal{D}})$ are well defined for *almost all* values of δ, that is for almost all times, momenta and unit vectors associated to the nodes of the evolution, and compatible with the hard core exclusion. The corresponding integrals in $d\delta$ are then extended over full measure regions over the sets compatible with the condition of hard core exclusion, so that we can substitute $\Omega_{j_i}(\cdots)$ with $\overline{\Omega}_{j_i}(\cdots)$ in the expression (3.10).

The so defined $V(\overline{\mathcal{D}})$ and $R(\mathcal{D})$ can be seen as operators respectively over the spaces of variables

$$\{\overline{\Delta}(\underline{x}_n; [0,t]) \mid n = 1, 2, \cdots, \underline{x}_n \in \Gamma_n^*, t > 0\}$$

and

$$\{\Delta(\underline{x}_n; [0,t]) \mid n = 1, 2, \cdots, \underline{x}_n \in \Gamma_n^*, t > 0\},$$

with values in some space of functions over $\Gamma_n^* \times (0, \infty), n = 1, 2, \cdots$ Notice that the integrals in t_i and $\hat{w}_i$ in (3.10) are over finite regions, while, in our assumptions, the integrals over $\hat{p}_i$ are controlled by the estimate

$$|\rho_{n+m}(x_1(\mathcal{D}), \cdots, x_{n+m}(\mathcal{D}))| \leq (\text{const}) \prod_{j=1}^{n} h_\beta(p_j) \prod_{j=1}^{m} h_\beta(\hat{p}_j),$$

which follows from (2.21) and conservation of energy, and

$$|W(\mathcal{D})| \leq \left(2a^2 \sqrt{\sum_{j=1}^{n} p_j^2 + \sum_{j=1}^{m} \hat{p}_j^2}\right)^m .$$

Hence the integrals in (3.10) are absolutely convergent, they define a measurable function over Γ_n for any $t > 0$ and, using $|p|^q h_\beta(p)/h_{\beta'}(p) \leq \text{const}$ for $q > 0, \beta' < \beta$, we have

$$|V(\overline{\mathcal{D}})| \leq C \prod_{j=1}^{n} h_{\beta'}(p_j)\ , \tag{3.12}$$

with $\beta' < \beta$ and C depending on N, a, Λ, t. Finally, oserve that $V(\overline{\mathcal{D}})$ is symmetric for exchange of particles $x_i \leftrightarrow x_j, i, j \in (1, \cdots, n)$, and simultaneous change $i \to$

$j, j \to i$ in the value of the node labels, so that certainly the sum over all trees $\sum_{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n;[0,t])} V(\overline{\mathcal{D}})$ is in $\mathcal{L}_n$.

In our main theorem we will prove that, starting with an initial density $f_N \in \mathcal{L}_N$, this sum does give the time evolution of the correlation functions.

Chapter 4

The evolution of correlation functions

In what follows we present our main theorem. After the statement of the theorem and some general comment, we derive the usual BBGKY hierarchy of equations (Section 4.1). Finally, we present also an extension of the result to measures of grand canonical type (Section 4.2).

Theorem 4.0.1 *Let P be an initial measure with density $f_N \in \mathcal{L}_N$. Then for any $t > 0$, the time–evolved correlation functions are given by*

$$\rho_n(\underline{x}_n, t) = \sum_{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n;[0,t])} V(\overline{\mathcal{D}}) \, , \qquad n \in \mathbb{N} \, , \tag{4.1}$$

almost everywhere in Γ_n. For any chosen version of $f_N(t), \rho_n(t)$ satisfying (2.19) and (2.20) over the whole sets $\hat{\Gamma}_n$, the expansion holds for all $\underline{x}_n \in \hat{\Gamma}_n$ and $t > 0$.

In reference [45] this formula is called the *"time–integrated form of the BBGKY hierarchy"*. Actually it is the complete *expansion* of the $n-$th correlation function at time t in terms of the higher order ($n+m,\ m \geq 0$) correlation functions at time zero. The number of terms in the sum is of course finite.

Remembering what has been said next to (3.1), we may define a measure $d\delta$ on $\Delta(\underline{x}_n; [0,t])$ as the counting measure with respect to the discrete variables $m, j_1, \dots, j_m$, and the Lebesgue measure with respect to the variables

$$t_1, \dots, t_m, \hat{p}_1, \dots, \hat{p}_m, \hat{w}_1, \dots, \hat{w}_m.$$

With these notations we can say that $R(\mathcal{D}) = R(\underline{x}_n, \delta)$ is a $d\delta-$summable function on $\Delta(\underline{x}_n; [0,t])$ for all t and almost all $\underline{x}_n \in \Gamma_n$, and we can rewrite (4.1) as an integral over collision histories:

$$\rho_n(\underline{x}_n, t) = \int_{\Delta(\underline{x}_n;[0,t])} d\delta R(\underline{x}_n, \delta) \qquad n \in \mathbb{N} \tag{4.2}$$

almost surely in Γ_n.

Remarks.

(1) We do not need f_N and ρ_n to be *continuous along trajectories* of $T_t^{(n)}$, that is we do not need

$$\lim_{s\to 0} f_N(T_s^{(N)}(x_1, \cdots, x_N)) = f_N(x_1, \cdots, x_N) \tag{4.3}$$

for a.a. $\underline{x}_N \in \Gamma_N$, where both the limits from the future and the past are understood. In particular, our initial density can distinguish between pre–collisional and post–collisional configurations (which can not be true if we assume for instance (4.3) on all Γ_n^*). It is easy to show (see [45]) that, if the continuity along trajectories is assumed to be valid for f_N, then the Liouville Equation (2.19) together with some integrable bound on f_N imply that: *(i)* the same continuity property is also valid for $f_N(t)$ and for $\rho_n(t)$ at any time $t \geq 0$; *(ii)* for almost all $\underline{x}_n$ the map $t \to \rho_n(\underline{x}_n, t)$ is continuous. All these properties, even if assumed, would be not helpful in the discussions of the present paper. In [45] and in [23] the continuity along trajectories is used to derive the series expansion (4.1).

(2) The bound (3.12) follows from rough estimate of the right hand side of (3.10), as already explained. That is sufficient for our purposes. From the proof of the theorem it will be clear that the bound (2.17) could even be substituted with a weaker one, since it is just needed to ensure absolute convergence of the integrals in (3.10). Our choice of the decay behavior for high momenta is the same used in the careful estimate of [27] of the right hand side of (3.10) (see the details in [24]), necessary to perform the Boltzmann–Grad limit: if the correlation functions satisfy $|\rho_n(\underline{x}_n)| \leq$ $\mathrm{c}(Nz)^n \prod_{j=1}^n h_\beta(p_j)$ for some $c, z, \beta > 0$, then the right hand side of (4.1) is bounded by $|\sum_{m\geq 0} \sum_{\overline{\mathcal{D}}\in\overline{\Delta}^{(m)}(\underline{x}_n;[0,t])} V(\overline{\mathcal{D}})| \leq c'(Nz')^n \prod_{j=1}^n h_{\beta'}(p_j) \sum_{m\geq 0}(\mathrm{const}\cdot Na^2 zt)^m$ for some $c', \beta' < \beta$ and $z' > z(\beta'/\beta)^{3/2}$ (here $\overline{\Delta}^{(m)}(\underline{x}_n; [0,t])$ is the subset of trees with m nodes). This ensures convergence for $N \to \infty, Na^2$ fixed, at least for sufficiently small t.

(3) Our result is actually stronger than the one obtained in [45] via density arguments, which is the same expansion integrated over every Borel set in Γ_n (and corresponds to the first statement in our theorem). We know that there exists a full measure subset of the phase space where the dynamics of the hard sphere system exists for all times (Proposition 2.1.1). Theorem 4.0.1 recovers this property

for the evolution of correlation functions: the expansion (4.1) is valid for all times in $\hat{\Gamma}_n$, that is a full measure subset of Γ_n, and invariant under the flow. This subset – see the definition of $\hat{\Gamma}_n$ in Eq. (2.14) – has not been characterized in a constructive manner: this would depend on details of the dynamics that have not been investigated. However, it will be clear from the proof that $\hat{\Gamma}_n$ is the maximal subset of the phase space where the result can be derived for all times. In particular, the second statement of our theorem is still true if we replace $\hat{\Gamma}_n$ with any full measure invariant subset of it, say $\mathcal{H}_n$, satisfying the following "chain property": if $\underline{x}_n \in \mathcal{H}_n$, then $(\underline{x}_n, \underline{y}_k) \in \mathcal{H}_{n+k}$ for almost all $\underline{y}_k \in \Gamma_k(\underline{x}_n)$.

(4) Choose a version of $f_N(t), \rho_n(t)$ satisfying (2.19) and (2.20) in a set $\mathcal{H}_n \subseteq \hat{\Gamma}_n$ (it is sufficient $\mathcal{H}_n \subseteq \Gamma_n^\dagger$) as described in the previous remark. Call (remember definitions (2.5), (2.6) and (2.7))

$$\mathcal{H}_n^{(+)} = \mathcal{H}_n \setminus (\Phi_n^- \cup \Psi_n^-) \ , \tag{4.4}$$

and notice that $\mathcal{H}_n^{(+)}$ is mapped by $T_t^{(n)}$ onto $\mathcal{H}_n$ for $t > 0$. Then, for all $\underline{x}_n \in \mathcal{H}_n^{(+)}$, we can write

$$\begin{aligned} & f_N(T_t^{(N)}(\underline{x}_N), t) = f_N(\underline{x}_N) \ , \\ & \rho_n(T_t^{(n)}(\underline{x}_n), t) = N \dots (N-n+1) \\ & \qquad \cdot \int_{\Gamma_{N-n}(T_t^{(n)}(\underline{x}_n))} dy_{n+1} \dots dy_N f_N(T_t^{(n)}(\underline{x}_n), dy_{n+1} \dots dy_N, t) \ , \end{aligned} \tag{4.5}$$

for all times $t > 0$. The converse is also true. Here the restriction to $\mathcal{H}_n^{(+)}$ corresponds to the conventional $+$ sign used in writing the Liouville Equation (2.19). In the next section we will use the above formula as a starting point to derive the integro–differential BBGKY equations.

(5) Theorem 4.0.1 and Lemma A.0.1 of Appendix A immediately imply that, for any chosen version satisfying (4.5) in $\hat{\Gamma}_n^{(+)}$, the identity (4.1) holds for every time over almost all $\partial\Gamma_n$.

(6) Formulas (4.1) and (4.2) suggest an interpretation of the contribution of a collision history to the right hand side in terms of constructive or destructive correlation effects of the "external" particles (i.e. those different from $(1, \cdots, n)$) on particles $(1, \cdots, n)$ during the time interval $[0, t]$. Consider for instance the history $(\underline{x}_n, \delta_1) \equiv (\underline{x}_n, 1, j_1, t_1, \hat{p}_1, \hat{w}_1)$ of Figure 3.3. This gives a positive or negative contribution to the right hand side of (4.1) depending on the sign of the weight factor $W_1(\underline{x}_n, \delta)$ associated to its node. In the first case, $W_1(\underline{x}_n, \delta) > 0$, the (only) external particle $n+1$ appears in an outgoing collision with particle j_1: its effect on particles $(1, \cdots, n)$ is that of *creating* the configuration $(x_1, \dots, x_n)$ at time t,

in the sense that if we forgot the interaction effect of particle $n+1$ on particle j_1 at time t_1 (thus modifying the trajectory drawn by the collision history), then by evolving forward in time we would not get $(x_1, \ldots, x_n)$ at time t. In the other case, $W_1(\underline{x}_n, \delta) < 0$, the particle $n+1$ appears in an ingoing collision with particle j_1: its effect on particles $(1, \cdots, n)$ is that of *annihilating* the configuration $(x_1, \ldots, x_n)$ at time t, in the sense that if we took into account the interaction effect of particle $n+1$ on particle j_1 at time t_1 (thus modifying the trajectory drawn by the collision history), then by evolving forward in time we would not get $(x_1, \ldots, x_n)$ at time t. More generally, in any tree, we can say that a node with positive weight factor describes a collision that creates, in the ordinary verse of time (that is going towards the root) a particle entering the next node of the tree – or entering the root if the node is the last one (i.e. creating $\underline{x}_n$ at time t); while a node with negative weight factor describes the annihilation of such a particle. It is then clear why, for instance, in trees with two nodes, two annihilation weight factors (negative) correspond to a net positive contribution to the right hand side of (4.1), two weight factors of different type (one positive and the other negative) to a net negative contribution, and so on.

4.1 The BBGKY hierarchy

We want to show here how the usual BBGKY hierarchy of integro–differential equations is recovered from the expansion (4.1). We present below the bulk of this derivation and refer to the appendices for some technical details. We begin by fixing a version of the density and the correlation functions satisfying (2.19) and (2.20), for simplicity, on the whole $\hat{\Gamma}_n$, so that Eq. (4.5) holds over all $\hat{\Gamma}_n^{(+)}$ and for all $t > 0$ (everything that follows would hold also replacing $\hat{\Gamma}_n$ with any subset $\mathcal{H}_n$: see Remarks 3 and 4 in the previous section). As we will see, starting from that formula it is easy to obtain informations about the function of time

$$t \longrightarrow \rho_n(T_t^{(n)}(x_1, \cdots, x_n), t) , \tag{4.6}$$

and its derivative, without additional assumptions on the initial measure. To begin with, it can be shown that, for any n and all $\underline{x}_n \in \hat{\Gamma}_n^{(+)}$ (or $\Gamma_n^{\dagger(+)}$), the function is *continuous* for every $t > 0$ – see Appendix D.

Secondly, we can rewrite the expansion (4.1) in a resummed form, which is convenient to obtain informations about the derivative, as explained in the following.

Fix $n < N$, and rewrite the expansion (4.1) as

$$\begin{aligned}
\rho_n(\underline{x}_n, t) &= \rho_n(T^{(n)}_{-t+}(x_1, \cdots, x_n)) \\
&+ \sum_{j_1=1}^{n} \int_0^t dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j_1}(T^{(n)}_{-t+t_1+}(\underline{x}_n),\hat{p}_1)} d\hat{w}_1 a^2 \hat{w}_1 \cdot (\hat{p}_1 - p_{j_1}(t_1; \underline{x}_n, \delta_1)) \\
&\cdot \rho_{n+1}\left(T^{(n+1)}_{-t_1+}\left(T^{(n)}_{-t+t_1+}(\underline{x}_n), q_{j_1}(t_1; \underline{x}_n, \delta_1) + a\hat{w}_1, \hat{p}_1\right)\right) + \sum_{\substack{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n;[0,t]) \\ m(\overline{\mathcal{D}})>1}} V(\overline{\mathcal{D}}) ,
\end{aligned} \tag{4.7}$$

for $\underline{x}_n \in \hat{\Gamma}_n$, where $(\underline{x}_n, \delta_1)$ is the tree with one node in Figure 3.3, and $m(\overline{\mathcal{D}})$ is the number of nodes of $\overline{\mathcal{D}}$. Remind that we can always substitute Ω_{j_1} with $\overline{\Omega}_{j_1}$ in the above expression (see Remark 3 in the previous section). In formula (4.7) we wrote explicitly the lowest order terms (zero–nodes and one–node trees) of the expansion. Since we restrict to $\underline{x}_n \in \mathcal{K}_n$, in the integrals corresponding to the one–node trees we may use again Equation (4.1) to substitute $\rho_{n+1}(\cdot, 0)$ with $\rho_{n+1}(\cdot, t_1)$: it follows that the second term in the right hand side of (4.7) is equal to

$$\begin{aligned}
&\sum_{j_1=1}^{n} \int_0^t dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j_1}(T^{(n)}_{-t+t_1+}(\underline{x}_n),\hat{p}_1)} d\hat{w}_1 a^2 \hat{w}_1 \cdot (\hat{p}_1 - p_{j_1}(t_1; \underline{x}_n, \delta_1)) \\
&\qquad \cdot \rho_{n+1}\left(T^{(n)}_{-t+t_1+}(\underline{x}_n), q_{j_1}(t_1; \underline{x}_n, \delta_1) + a\hat{w}_1, \hat{p}_1, t_1\right) \\
&- \sum_{j_1=1}^{n} \int_0^t dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j_1}(T^{(n)}_{-t+t_1+}(\underline{x}_n),\hat{p}_1)} d\hat{w}_1 a^2 \hat{w}_1 \cdot (\hat{p}_1 - p_{j_1}(t_1; \underline{x}_n, \delta_1)) \\
&\qquad \cdot \sum_{\substack{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1}(t_1;\underline{x}_n,\delta_1);[0,t_1]) \\ m(\overline{\mathcal{D}})>0}} V(\overline{\mathcal{D}}) .
\end{aligned} \tag{4.8}$$

The second line of the last formula gives all the trees with at least two nodes, i.e. $-\sum_{\substack{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n;[0,t]) \\ m(\overline{\mathcal{D}})>1}} V(\overline{\mathcal{D}})$. Hence for $\underline{x}_n \in \hat{\Gamma}_n$ we have found

$$\begin{aligned}
\rho_n(\underline{x}_n, t) &= \rho_n(T^{(n)}_{-t+}(x_1, \cdots, x_n)) \\
&+ \sum_{j_1=1}^{n} \int_0^t dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j_1}(T^{(n)}_{-t+t_1+}(\underline{x}_n),\hat{p}_1)} d\hat{w}_1 a^2 \hat{w}_1 \cdot (\hat{p}_1 - p_{j_1}(t_1; \underline{x}_n, \delta_1)) \\
&\cdot \rho_{n+1}\left(T^{(n)}_{-t+t_1+}(\underline{x}_n), q_{j_1}(t_1; \underline{x}_n, \delta_1) + a\hat{w}_1, \hat{p}_1, t_1\right)
\end{aligned} \tag{4.9}$$

(which is again an absolutely convergent integral). Formula (4.9) is the *resummed* form of the expansion for the correlation functions, in the sense that iterating the equation $N - n$ times we are back to the Equation (4.1).

Recalling the continuity property stated at the beginning of the section, we can write also

$$\rho_n(T^{(n)}_t(\underline{x}_n), t) = \rho_n(\underline{x}_n) + \int_0^t dt_1 \, (Q_{n+1}\rho_{n+1}) \, (T^{(n)}_{t_1+}(\underline{x}_n), t_1) \tag{4.10}$$

for $\underline{x}_n \in \hat{\Gamma}_n^{(+)}$, where the *collision operator* Q_{n+1} acting on the time–evolved correlation function, is defined by

$$(Q_{n+1}\rho_{n+1})(\underline{x}_n, t) \tag{4.11}$$
$$= \sum_{j=1}^{n} a^2 \int_{\mathbb{R}^3} d\hat{p} \int_{\overline{\Omega}_j(\underline{x}_n)} d\hat{w}\hat{w} \cdot (\hat{p} - p_j)\, \rho_{n+1}(\underline{x}_n, q_j + a\hat{w}, \hat{p}, t) \ .$$

over $\hat{\Gamma}_n \times [0, \infty)$. The integrand in (4.10) is a measurable function in the variable t_1 for all $\underline{x}_n \in \mathcal{K}_n$, while, for all t, the definition (4.11) can be extended to Γ_n, providing a function in the space $\mathcal{L}_n$. The definition is, in our assumptions, independent on the chosen version in the sense that, if $\tilde{\rho}_{n+1}(\underline{x}_{n+1}) = \rho_{n+1}(\underline{x}_{n+1})$ for almost all $\underline{x}_{n+1} \in \Gamma_{n+1}$, then the same is true for the time–evolved functions for all $t \geq 0$ (see (4.5)) and, by the continuity property stated in the second part of Lemma D.0.1, the two functions coincide also for almost all $(\underline{x}_{n+1}, t) \in \partial\Gamma_{n+1} \times [0, \infty)$ (see also the final paragraph in the proof of Lemma A.0.1), so that $Q_{n+1}\rho_{n+1} = Q_{n+1}\tilde{\rho}_{n+1}$ for almost all $(\underline{x}_n, t) \in \Gamma_n \times [0, \infty)$.

Formula (4.10) shows that $t \longrightarrow \rho_n(T_t^{(n)}(\underline{x}_n), t)$ is also absolutely continuous. As a conclusion, we can state

Corollary 4.1.1 *Given an initial measure with density $f_N \in \mathcal{L}_N$, and $f_N(t), \rho_n(t)$ satisfying (2.19) and (2.20) on $\hat{\Gamma}_n$, the function $t \longrightarrow (Q_{n+1}\rho_{n+1})(T_t^{(n)}(\underline{x}_n), t)$ is measurable and the correlation functions satisfy*

$$\frac{d}{dt}\rho_n(T_t^{(n)}(\underline{x}_n), t) = (Q_{n+1}\rho_{n+1})(T_t^{(n)}(\underline{x}_n), t) \ , \qquad n \in \mathbb{N} \, , \tag{4.12}$$

for all $\underline{x}_n \in \hat{\Gamma}_n^{(+)}$ and almost all $t > 0$.

The subsets of the phase space involved in the assertion of the lemma have full Lebesgue measure. Remind that $\hat{\Gamma}_n^{(+)}$ is mapped by $T_t^{(n)}$ onto $\hat{\Gamma}_n$ for $t > 0$.

Remarks.

(1) If, additionally, $f_N \in C(\Gamma_n)$ then, for all $\underline{x}_n \in \hat{\Gamma}_n \setminus \partial\Gamma_n$ and almost all $t > 0$, it could be proven that the right hand side is continuous in t. The boundary $\partial\Gamma_n$ is discarded as it contains the (possible) points of discontinuity along trajectories of the time–zero correlation functions.

(2) We did not used the continuity along trajectories of the correlation functions. Thus the result strengthens the analogous in [7]. Weaker versions of the hierarchy have been already proved without the assumption of continuity along trajectories, see [23] or [7].

(3) Unlike the series solution (4.1), the BBGKY hierarchy in differential form explicitly involves restrictions of the correlation functions to sets of codimension 1:

this has made crucial the property of existence of the flow on the collision surfaces (second statement in Proposition 2.1.1).

4.2 Indefinite number of particles

Finally, we can extend the result of Theorem 4.0.1 to a more general class of measures with non definite (but finite) number of particles. We follow [45] for this purpose. Consider the grand canonical phase space

$$\Gamma = \cup_{n\geq 0}\Gamma_n \ . \tag{4.13}$$

Then it will be $\Gamma_n = \emptyset$ for n larger then $[3|\Lambda|/4\pi a^3]$, because of the hard core exclusion.

Call $\mathcal{L}$ the space of measurable functions $f : \Gamma \to \mathbb{R}, f = \{f_n\}_{n=0}^{\infty}$, symmetric in the particle labels ($f_n(\Pi(x_1, \dots, x_n)) = f_n(x_1, \dots, x_n)\ \forall n$, for any permutation Π), and having the boundedness property

$$|f_n(x_1, \dots, x_n)| \leq A \prod_{j=1}^{n} (z h_\beta(p_j)) \ , \tag{4.14}$$

on Γ_n, for some $A, z, \beta > 0$. We can put $f_n = 0$ for $n > [3|\Lambda|/4\pi a^3]$. If P denotes a measure on Γ with density $f \in \mathcal{L}$ with respect to Lebesgue measure, then the time–evolved measure at time t has a density $f(t) \in \mathcal{L}$ given by

$$f_n(x_1, \dots, x_n, t) = f_n(T^{(n)}_{-t+}(x_1, \dots, x_n)) \ , \qquad n \in \mathbb{N} \tag{4.15}$$

almost everywhere in Γ_n.

Given $f \in \mathcal{L}$, we define the *correlation function vector* $\rho : \Gamma \longrightarrow \mathbb{R}, \rho = \{\rho_n\}_{n=0}^{\infty}$ by

$$\rho_n(x_1, \dots, x_n, t) = \sum_{k=0}^{\infty} \frac{1}{k!} \int_{\Gamma_k(x_1,\dots,x_n)} dx_{n+1} \dots dx_{n+k} f_{n+k}(x_1, \dots, x_{n+k}, t) \ , \tag{4.16}$$

where equality is in the space $\mathcal{L}_n$. Again we have that $\rho \in \mathcal{L}$ and furthermore, the map defined by (4.16) has the inverse

$$f_n(x_1, \dots, x_n, t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{\Gamma_k(x_1,\dots,x_n)} dx_{n+1} \dots dx_{n+k} \rho_{n+k}(x_1, \dots, x_{n+k}, t) \tag{4.17}$$

The following extension will be an immediate consequence of the analysis developed in the next section.

Corollary 4.2.1 *Let P be an initial measure on Γ with density $f \in \mathcal{L}$. Then for any $t > 0$, the time–evolved correlation functions are given by*

$$\rho_n(\underline{x}_n, t) = \sum_{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n;[0,t])} V(\overline{\mathcal{D}}) \, , \qquad n \in \mathbb{N} \, ,$$

almost everywhere in Γ_n. For any chosen version of $f_n(t), \rho_n(t)$ satisfying (4.15) and (4.16) over the whole sets $\hat{\Gamma}_n$, the expansion holds for all $\underline{x}_n \in \hat{\Gamma}_n$ and $t > 0$.

(Here $\hat{\Gamma}_n$ is defined as in (2.14) with $k \geq 1$.)

Each term in the sum in Equation (4.16) may be dealed with the procedure explained in Chapter 5. This leads directly to a tree expansion of the type in the right hand side of (4.1), in which the value of the tree, say $\tilde{V}(\overline{\mathcal{D}})$, is computed in a slightly different way in terms of the density function f. To evaluate $\tilde{V}(\overline{\mathcal{D}})$, follow the rules introduced in Section 3.3, substituting formula (3.8) with

$$\begin{aligned} \frac{1}{(k-m)!} \int_{\Gamma_{k-m}(x_1(\mathcal{D}),\cdots,x_{n+m}(\mathcal{D}))} & dx_{n+m+1} \cdots dx_{n+k} \\ & \cdot f_{n+k}\left(x_1(\mathcal{D}), \cdots, x_{n+m}(\mathcal{D}), x_{n+m+1}, \cdots, x_{n+k}\right) \, . \end{aligned} \tag{4.18}$$

Performing the sum over k, that is $\sum_{k\geq m}^{\infty}$, and using (4.16), we obtain the corollary.

Chapter 5

Proof of Theorem 4.0.1

In this chapter we prove our main result. We shall proceed by induction on n: supposing the statement of the theorem true for the function ρ_{n+1}, we derive the expansion for the ρ_n by integrating a single degree of freedom. The rigorous integration procedure is rather technical but, in spite of lengthiness of formulas (for which sometimes we refer to the appendices), the integration of a degree of freedom in a single term (tree) of the expansion admits a quite simple graphical representation in terms of "extraction" of subtrees and "reattachment" of extracted subtrees. These operations over trees are introduced in Section 5.1, while the graphical integration rules are summarized in Proposition 5.2.1 in Section 5.2. Along the proof of the proposition, in the same section, we present the analytical operations depicted by the operations over trees: they consist essentially in appropriate partitioning of the integration domain and representation of its subsets. However, this is not sufficient: to prove the proposition it is also essential to notice that a certain class of collision histories gives a net null contribution to the integral, because of one by one cancellations. This will be done in Lemma 5.2.1. Finally, in Section 5.3 we conclude the proof of the theorem, by discussing the summation of all the graphical terms obtained through the integration procedure.

5.1 Tools: manipulation of trees

The integration of degrees of freedom will be described by a manipulation of the trees involving "pruning", "extraction" and "growth" operations, for which we will need some more notations. As in the previous sections, we will indicate with $m = m(\overline{\mathcal{D}}) = m(\overline{\delta})$ (or $m(\mathcal{D})$) the number of nodes of the tree $\overline{\mathcal{D}} = (\underline{x}_n, \overline{\delta})$ (collision history $\mathcal{D}$), and with $j_k = j_k(\overline{\mathcal{D}}) = j_k(\overline{\delta})$ ($j_k(\mathcal{D})$) the variable defined in (3.2). Moreover, we will call $\overline{\Delta}_{n,m}$ the set of trees in $\overline{\Delta}(\underline{x}_n; [0,t])$ with m nodes and not specified time and initial configuration (no labels attached to the root); clearly an element $\overline{\mathcal{G}} \in \overline{\Delta}_{n,m}$ is identified with a set of variables $(n, m, j_1, \cdots, j_m)$, see (3.3). For the trivial tree, that is the only one belonging to $\overline{\Delta}_{1,0}$, we will use the symbol $\overline{\mathcal{T}}$.

Given $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t])$, order its nodes from left to right with the index k as in Chapter 3. We name $\overline{\mathcal{D}}_k \in \overline{\Delta}_{1,m'}$ the *subtree generated* in the node number k, and we call $\overline{\mathcal{D}}_{/k} \in \overline{\Delta}(\underline{x}_n; [0,t])$ the tree obtained from $\overline{\mathcal{D}}$ by *pruning* $\overline{\mathcal{D}}_k$ (it will be $m' \leq m(\overline{\mathcal{D}}) - 1$).

Now we extend these definitions to the case $k = 0$. We call $\overline{\mathcal{D}}_{0;j}, j = 1, \cdots, n$ the tree in $\overline{\Delta}_{1,m'}$ obtained from $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t])$ by pruning all the subtrees $\overline{\mathcal{D}}_k$ such that the node k lies in the root line and has a label $j_k \neq j$ (it will be $m' \leq m(\overline{\mathcal{D}})$). Similarly, we call $\overline{\mathcal{D}}_{/0;j}, j = 1, \cdots, n$ the tree in $\overline{\Delta}(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_n; [0,t])$ obtained from $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t])$ by pruning all the subtrees $\overline{\mathcal{D}}_k$ such that the node k lies in the root line and has a label $j_k = j$. Notice that in the case there is no node label with value j, it is $m' = 0$, $\overline{\mathcal{D}}_{0;j} = \overline{\mathcal{T}}$, and $\overline{\mathcal{D}}_{/0;j}$ is the tree in $\overline{\Delta}(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_n; [0,t])$ which is identical to $\overline{\mathcal{D}}$ except for the label attached to the root, i.e. $\overline{\mathcal{D}}_{/0;j} = (x_1, \cdots, x_{j-1}, x_{j+1}, \cdots, x_n, \overline{\delta})$ if $\overline{\mathcal{D}} = (\underline{x}_n, \overline{\delta})$.

We can also visualize the trees $\overline{\mathcal{D}}_{0;j}$ in the following manner. Imagine that the root line of $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0,t])$ is composed by n coincident identical lines, numbered from 1 to n and associated to the particles of the initial configuration $\underline{x}_n$. The $j-$th of these line, $j = 1, \cdots, n$, is thought as attached only to the subtrees generated in the nodes of the root line carrying a node label with value j. Then we can say that the subtree $\overline{\mathcal{D}}_{0,j}$, is obtained by *extraction* of the $j-$th line, together with the subtrees attached to it, from the tree $\overline{\mathcal{D}}$ (and by deleting decorations). The $j-$th line will become the root line of the extracted tree. What is left of the original $\overline{\mathcal{D}}$ after the extraction of $\overline{\mathcal{D}}_{0;j}$ and after deleting the root label x_j as well as the node labels with value j, is exactly the tree $\overline{\mathcal{D}}_{/0;j}$.

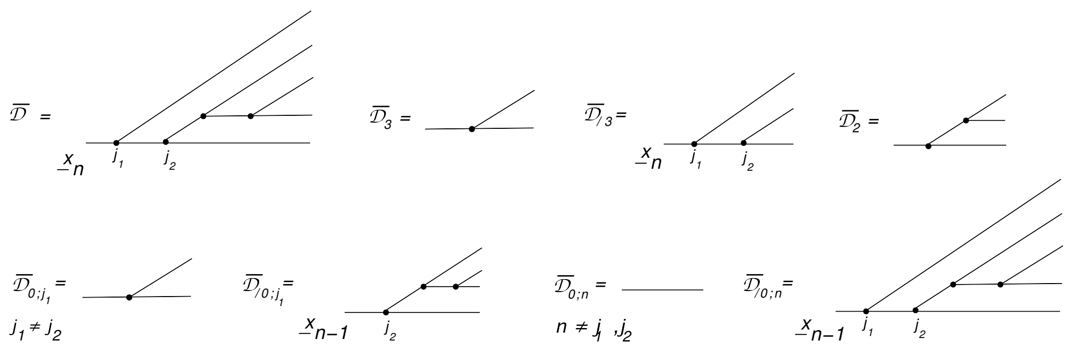

Figure 5.1. Notations for subtrees, pruned trees and extracted subtrees.

Finally, for $n \leq N$, we define the *composition of trees*

$$\circ_{\underline{k};i}, \underline{k} = (k_0, \cdots, k_q) \in \mathbb{Z}^{q+1}, 1 \leq k_0 < k_1 < \cdots < k_q,$$

by

$$\begin{aligned} &\circ_{k_0,\cdots,k_q;i} : \overline{\Delta}(\underline{x}_n;[0,t]) \times \overline{\Delta}_{1,q} \to \overline{\Delta}(\underline{x}_n;[0,t]) \\ &\overline{\mathcal{D}} \circ_{\underline{k},i} \overline{\mathcal{G}} = \overline{\mathcal{H}} \qquad \text{such that } \overline{\mathcal{H}}_{k_0} = \overline{\mathcal{G}},\ \overline{\mathcal{H}}_{/k_0} = \overline{\mathcal{D}}\ , \\ &\qquad\qquad\qquad \text{the nodes of } \overline{\mathcal{H}}_{k_0} \text{ have ordering} \\ &\qquad\qquad\qquad \text{numbers } k_1, \cdots, k_q \text{ in } \overline{\mathcal{H}}, \text{ and} \\ &\qquad\qquad\qquad \text{the label } j_{k_0} \text{ of } \overline{\mathcal{H}} \text{ is equal to } i\ , \\ &\qquad\qquad\qquad \text{for } k_q \leq m(\overline{\mathcal{D}}) + q + 1 \text{ and } 1 \leq i \leq n + k_0 - 1\ , \end{aligned} \tag{5.1}$$

and $\emptyset$ otherwise. This means simply that $\circ_{\underline{k};i}$ *grows* the tree $\overline{\mathcal{D}}$ by attaching to it the tree $\overline{\mathcal{G}}$ in such a way that:

1. the root of $\overline{\mathcal{G}}$ is attached to the root line of $\overline{\mathcal{D}}$ when $i \in (1, \cdots, n)$, and to the $r-$th line when $i = n + r, 1 \leq r \leq m(\overline{\mathcal{D}})$;

2. a node with ordering number k_0 is created in the previous operation;

3. the ordering numbers of the nodes of $\overline{\mathcal{G}}$ in the resulting tree are given by (from left to right) $k_1, \cdots, k_q, q = m(\overline{\mathcal{G}})$.

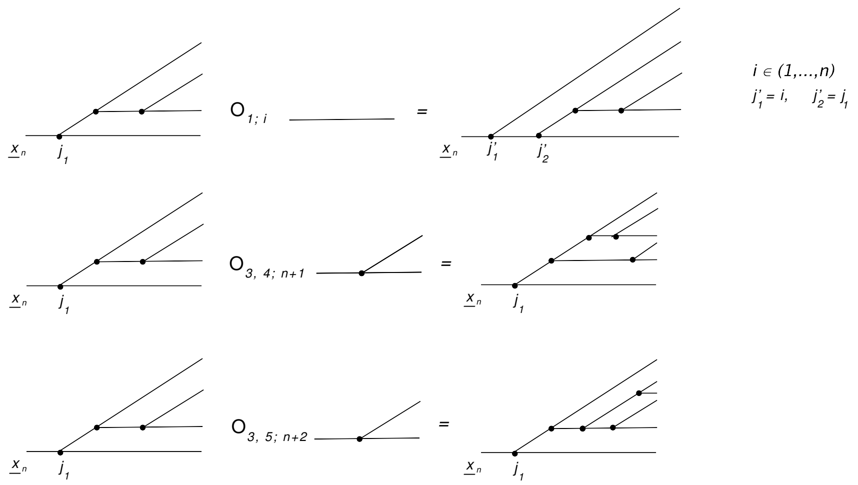

Figure 5.2. Examples of composition of trees: in $\overline{\mathcal{D}} \circ_{\underline{k};i} \overline{\mathcal{G}}$ the indices k_0, i indicate to which line of $\overline{\mathcal{D}}$ (and between which nodes) has to be attached the root of $\overline{\mathcal{G}}$, and the $k_1, \cdots, k_q$ indicate how to order the q nodes of the subtree $\overline{\mathcal{G}}$ in the resulting tree.

5.2 Integrating a degree of freedom

Formula (4.1) is trivial for $n > N$, while for $n = N$ it gives, graphically,

$$\rho_N(\underline{x}_N, t) = \quad \underline{x}_N \, \rule{3cm}{0.4pt} = \rho_N(T^{(N)}_{-t+}(\underline{x}_N)) \tag{5.2}$$

a.e. in Γ_N, which is implied by (2.20) and (2.19).

We shall proceed by induction on n to prove the theorem: from (2.20) follows

$$\rho_n(\underline{x}_n, t) = \frac{1}{N-n} \int_{\Gamma_1(\underline{x}_n)} dx_{n+1} \rho_{n+1}(\underline{x}_n, x_{n+1}, t) \; , \qquad 1 \le n < N \; , \tag{5.3}$$

so that assuming (4.1) valid for ρ_{n+1} we can write

$$\rho_n(\underline{x}_n, t) = \frac{1}{N-n} \int_{\Gamma_1(\underline{x}_n)} dx_{n+1} \sum_{\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1};[0,t])} V(\overline{\mathcal{D}}) \tag{5.4}$$

a.e. in Γ_n, or exactly in $\hat{\Gamma}_n$ if we are assuming (2.19) and (2.20) to hold over it: *this will be understood in what follows from now on.* Then we need to explain what is the result when we integrate the single degree of freedom in a tree of the set $\overline{\Delta}(\underline{x}_{n+1}; [0, t])$, i.e. we have to compute

$$I(\overline{\mathcal{D}}) = I(\overline{\mathcal{D}})(\underline{x}_n, t) := \int_{\Gamma_1(\underline{x}_n)} dx_{n+1} V(\underline{x}_{n+1}, \overline{\delta}) \; , \qquad \overline{\mathcal{D}} = (\underline{x}_{n+1}, \overline{\delta}) \in \overline{\Delta}(\underline{x}_{n+1}; [0, t]) \tag{5.5}$$

for a set of $\underline{x}_n$ of full measure in Γ_n. Notice that the integral in the above formula is well defined as a measurable function over Γ_n, see the final comments in Section 3.3.

The computation of (5.5) will be the main part of the proof, and the rest of this section. After that, we must just sum the result over all the trees of the family $\overline{\Delta}(\underline{x}_{n+1}; [0, t])$.

5.2.1 Integration of a degree of freedom in a single tree

Given $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1}; [0, t])$, and selected a particle $j \in (1, \cdots, n+1+m(\overline{\mathcal{D}}))$, call

$$q^{(j)}_1, q^{(j)}_2, \cdots \tag{5.6}$$

the ordering number of the nodes, in $\overline{\mathcal{D}}$, that belong also to the subtree with root line given by the line associated to particle j: $\overline{\mathcal{D}}_{0;j}$ in the case $j \in (1, \cdots, n+1)$, or $\overline{\mathcal{D}}_k$ in the case $j = n+1+k, k > 0$.

Write $\underline{q}^{(j)} = (q^{(j)}_1, q^{(j)}_2, \cdots)$. Define a variable $l^* = l^*(\overline{\mathcal{D}})$ by

$$l^* = \begin{cases} q^{(n+1)}_1 & \text{if } m(\overline{\mathcal{D}}_{0;n+1}) \ge 1 \\ m(\overline{\mathcal{D}}) + 1 & \text{if } m(\overline{\mathcal{D}}_{0;n+1}) = 0 \end{cases} \; . \tag{5.7}$$

To avoid confusion, indicate with the symbol $a_{i,j}$ the Kronecker delta. Finally, abbreviate $\underline{q}_+^{(n+1)} = (q_1^{(n+1)}+1, q_2^{(n+1)}+1, \cdots, q_{m(\overline{\mathcal{D}}_{0;n+1})}^{(n+1)}+1)$.

The bulk of the theorem is contained in the following assertion.

Proposition 5.2.1 *For any $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1}; [0,t]), 1 \le n \le N-1, t > 0$ and almost all $\underline{x}_n \in \Gamma_n$, the integral $I(\overline{\mathcal{D}})(\underline{x}_n, t)$ is given by the following sum of values of trees of $\overline{\Delta}(\underline{x}_n; [0,t])$:*

$$I(\overline{\mathcal{D}}) = a_{m(\overline{\mathcal{D}}_{0;n+1}),0}\left(N-n-m(\overline{\mathcal{D}})\right)V(\overline{\mathcal{D}}_{/0;n+1}) \\ +\sum_{k\ge1}^{l^*}\sum_{i\ge1}^{n+k-1} V\left(\overline{\mathcal{D}}_{/0;n+1}\circ_{k,\underline{q}_+^{(n+1)};i}\overline{\mathcal{D}}_{0;n+1}\right). \tag{5.8}$$

Using the terminology introduced in Section 5.1, we can give the following graphical picture of Proposition 5.2.1. The nodes divide each line of a tree in segments that we shall call *branch intervals.* To compute $I(\overline{\mathcal{D}}), \overline{\mathcal{D}} = (\underline{x}_{n+1}, \overline{\delta}) \in \overline{\Delta}(\underline{x}_{n+1}; [0,t])$:

1. *extract* from $\overline{\mathcal{D}}$ the subtree $\overline{\mathcal{D}}_{0;n+1}$; what is left is $\overline{\mathcal{D}}_{/0;n+1}$.

2. *Reattach* $\overline{\mathcal{D}}_{0;n+1}$ through its root to any branch interval of $\overline{\mathcal{D}}_{/0;n+1}$, with the following care. The resulting tree will have the old $m(\overline{\mathcal{D}})$ nodes of the starting tree $\overline{\mathcal{D}}$, plus one new node to which the root of $\overline{\mathcal{D}}_{0;n+1}$ is attached: the reattachment must be done in such a way that the reciprocal order of the old nodes in the resulting tree is the same as it was in the original tree $\overline{\mathcal{D}}$.

3. If the new node lies on the root line, append to it a node label with value in the set $(1, \cdots, n)$.

4. Sum all the possible resulting trees found in points 2,3.

5. If $m(\overline{\mathcal{D}}_{0;n+1}) = 0$, add to the result of point 4 the tree obtained by *discarding* $\overline{\mathcal{D}}_{0;n+1} = \overline{\mathcal{T}}$, i.e. $\overline{\mathcal{D}}_{/0;n+1} = (\underline{x}_n, \overline{\delta})$, multiplied by a factor $(N-n-m(\overline{\mathcal{D}}))$.

Several examples are provided by Figure 5.3.

5.2.2 Proof of Proposition 5.2.1: first step

In this section and in the following we give an outline of the proof of Proposition 5.2.1: we refer to the appendices for the details.

We shall begin with a couple of general definitions that will be useful along the proof. Let $\mathcal{D} \in \Delta(\underline{x}_n; [0,t]), \mathcal{D} = (\underline{x}_n, \delta)$, with δ as in (3.3). Let $k \in (1, \cdots, m(\mathcal{D}))$, and denote $\mathcal{D}_{/\hat{w}_k}$ the collection of variables $\mathcal{D}$ deprived of variable $\hat{w}_k$. Similarly, $(\mathcal{E}_\mathcal{D})_{/k}(s)$ $((\mathcal{N}_\mathcal{D})_{/k}(s))$ will indicate the state (number) of particles of the evolution

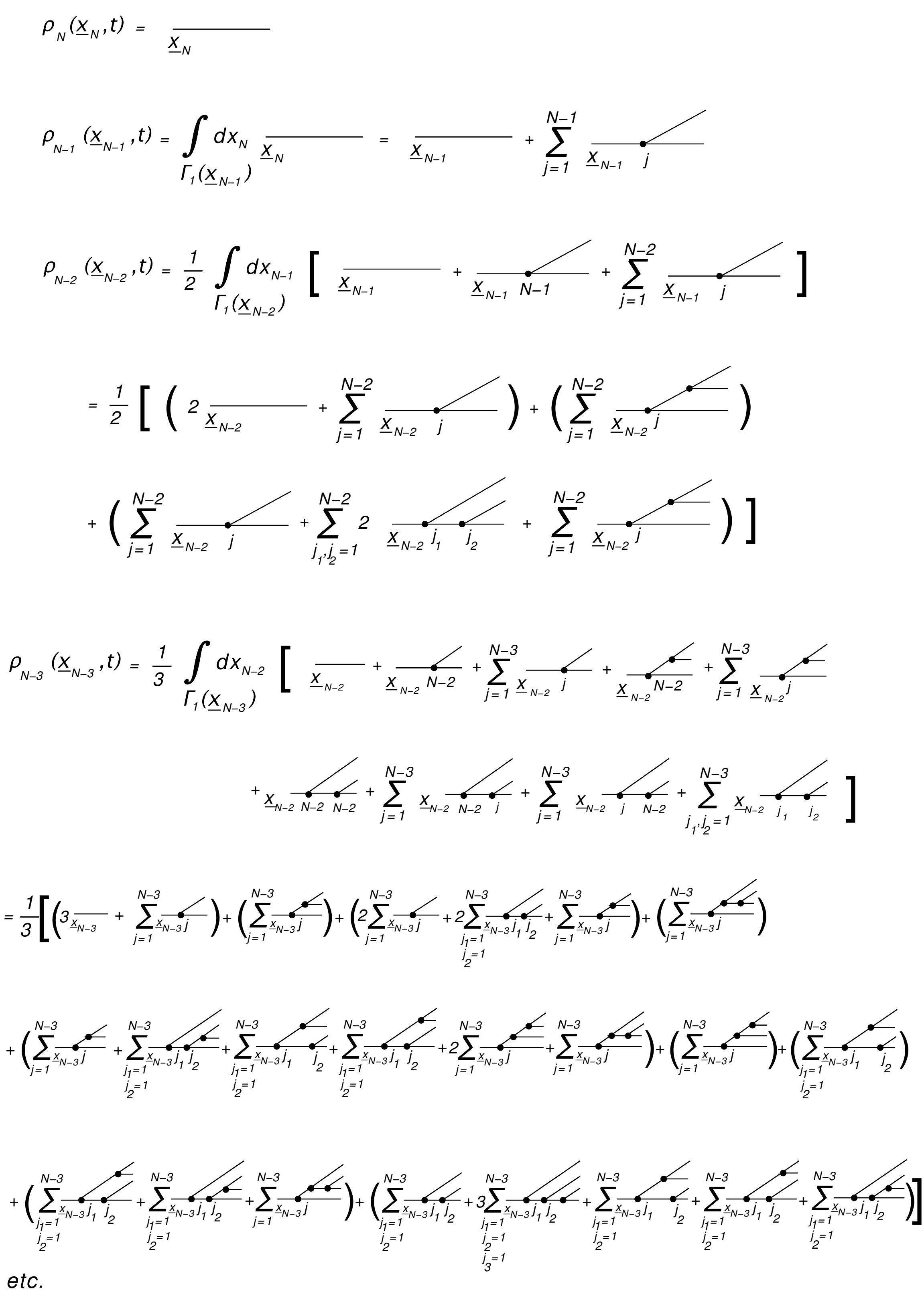

Figure 5.3. Integration of degrees of freedom: from Liouville equation to BBGKY hierarchy.

associated to $\mathcal{D}$ at time s, *forgetting* (when it is present) particle $n+k$. We define two subsets of the unit sphere surface by

$$\begin{aligned}\Omega^{(*)}_{j_k\pm}(\mathcal{D}_{/\hat{w}_k}) := \Big\{ & \hat{w}_k \text{ such that } \mathcal{D}\in\Delta(\underline{x}_n;[0,t]) \text{ and} \\ & \Big((\mathcal{E}_{\mathcal{D}})_{/k}(t_k\pm s), T^{(1)}_{\pm s}(q_{j_k}(t_k;\mathcal{D})+a\hat{w}_k,\hat{p}_k)\Big)\in\Gamma_{(\mathcal{N}_{\mathcal{D}})_{/k}(t_k\pm s)+1} \\ & \forall s\in(0,\tau_\pm)\Big\}\ ,\end{aligned} \tag{5.9}$$

where $\tau_+ = t-t_k$ and $\tau_- = t_k - t_{q_1^{(n+k)}}$ (the condition of existence of the free dynamics is understood in the definition). That is, $\hat{w}_k\in\Omega^{(*)}_{j_k\pm}(\mathcal{D}_{/\hat{w}_k})$ ensures that particle $n+k$ moves freely with no collisions with the other particles of $\mathcal{E}_{\mathcal{D}}$ for all times (up to t) in the future (+ case) or up to the time, in the past, in which a new particle is created through a collision with $n+k$ (− case).

For future convenience, given $(\underline{x}_n,\overline{\delta})\in\overline{\Delta}(\underline{x}_n;[0,t])$, we introduce the *set of collision histories for fixed tree* $\overline{\delta}$, $\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])$, which is in one by one correspondence with the set of times, momenta and unit vectors with the constraints explained in the definition of collision history. We use the notation

$$\hat{\delta} = (t_1,\dots,t_m,\hat{p}_1,\dots,\hat{p}_m,\hat{w}_1,\dots,\hat{w}_m)\ , \tag{5.10}$$

$\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])\ni\mathcal{D}=(\underline{x}_n,\overline{\delta},\hat{\delta})$, and we define a measure $d\hat{\delta}$ on $\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])$ as the Lebesgue measure with respect to the variables $t_1,\dots,t_m,\hat{p}_1,\dots,\hat{p}_m,\hat{w}_1,\dots,\hat{w}_m$. The value of the tree can be written

$$V(\overline{\mathcal{D}}) = \int_{\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta} R(\underline{x}_n,\overline{\delta},\hat{\delta})\ . \tag{5.11}$$

The proof consists of two steps. In the first one, by using a careful subdivision of the integration region as well as appropriate changes of variables, we derive a formula which is the same as (5.8) except for the fact that the integrals over collision histories in the right hand side (hidden in the definition of V) are *restricted* to certain subsets. Namely, in the assumptions of the Proposition and using the notations

$$\begin{aligned}&\overline{\mathcal{D}} = (\underline{x}_{n+1},\overline{\delta})\ ,\\ &\overline{\mathcal{D}}_{/0;n+1}\circ_{k,\underline{q}_+^{(n+1)};i}\overline{\mathcal{D}}_{0;n+1} = (\underline{x}_n,\overline{\gamma}_{k,i})\ ,\end{aligned} \tag{5.12}$$

we can prove

$$\begin{aligned}I(\overline{\mathcal{D}}) = {}& a_{m(\overline{\mathcal{D}}_{0;n+1}),0}\Big(N-n-m(\overline{\mathcal{D}})\Big)V(\overline{\mathcal{D}}_{/0;n+1}) \\ & +\sum_{k\geq1}^{l^*}\sum_{i\geq1}^{n+k-1}\int_{\Delta^{(*)}_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i}R(\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i})\ ,\end{aligned} \tag{5.13}$$

for almost all $\underline{x}_n \in \Gamma_n$, where

$$\begin{aligned}
&\Delta^{(*)}_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t]) := \Delta^{(*)}_{\overline{\gamma}_{k,i}+}(\underline{x}_n;[0,t]) \cup \Delta^{(*)}_{\overline{\gamma}_{k,i}-}(\underline{x}_n;[0,t]) \qquad \text{(disjoint union)}\\
&\Delta^{(*)}_{\overline{\gamma}_{k,i}\pm}(\underline{x}_n;[0,t]) := \Big\{\hat{\gamma}_{k,i} \in \Delta_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t]),\ \text{with}\\
&\qquad \hat{\gamma}_{k,i} = \Big(t_1,\cdots,t_{m(\overline{\gamma}_{k,i})},\hat{p}_1,\cdots,\hat{p}_{m(\overline{\gamma}_{k,i})},\hat{w}_1,\cdots,\hat{w}_m(\overline{\gamma}_{k,i})\Big)\\
&\qquad \text{such that } \hat{w}_k \in \Omega^{(*)}_{j_k(\overline{\gamma}_{k,i})\pm}((\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i})_{/\hat{w}_k})\Big\}\,. \qquad (5.14)
\end{aligned}$$

In what follows we shall explain briefly and without formulas how this equation is derived, restricting for simplicity to the case $m(\overline{\mathcal{D}}_{0;n+1}) = 0$; the rigorous proof is in Appendix B. In $I(\overline{\mathcal{D}})$ we integrate over x_{n+1} an expression which is given by an integral over the collision histories $\mathcal{D}$ that are compatible with the tree $\overline{\mathcal{D}}$, of a function R which depends only on the evolution $\mathcal{E}_{\mathcal{D}}$ – see (5.5), (5.11). After interchanging these integrations, we can parametrize x_{n+1}, that is the state of particle $n+1$ of the evolution at time t, with the state of the same particle *outgoing* its *last* (in $[0,t]$) collision in $\mathcal{E}_{\mathcal{D}}$, when this collision exists. Such a state is described by the time of the last collision t^*, the index i indicating which particle undergoes the collision with the $n+1$–th, the unit vector $\hat{w}^* := a^{-1}(q_{n+1}(t^*;\mathcal{D}) - q_i(t^*;\mathcal{D}))$, and the momentum $\hat{p}^*$ of particle $n+1$ outgoing the collision (which is equal to p_{n+1}). Then, for x_{n+1} such that this collision exists, say with i, we change variable $x_{n+1} \longrightarrow (t^*,\hat{p}^*,\hat{w}^*)$: the resulting integrals $\int dt^* \int d\hat{p}^* \int_{\Omega^{(*)}_{i+}} d\hat{w}^*$ correspond to a new node that has to be added to $\overline{\mathcal{D}}$, while the Jacobian determinant produces the associated weight factor. The net effect is the value of a tree produced via operations 1 and 2 of the list at page 41, when the integrations associated to the new node are restricted to "*outcoming collisions* producing a particle that *does not collide* with the particles of the evolution for all times in the future up to time t".

We are left with the integral over x_{n+1} such that the last collision *does not* exist. There the integrand is composed by a weight function which is independent on x_{n+1} (since we are assuming also $m(\overline{\mathcal{D}}_{0;n+1}) = 0$), and a time–zero correlation function $\rho_{n+1+m(\overline{\mathcal{D}})}$ which depends on x_{n+1} only through its correspondent value at time zero $T^{(1)}_{-t+}(x_{n+1})$. Therefore, by changing variable $x_{n+1} \longrightarrow x'_{n+1} = T^{(1)}_{-t+}(x_{n+1})$ and *extending* the integration over the whole one particle phase space compatible with the state of the other particles of $\mathcal{E}_{\mathcal{D}}(0)$, we eliminate completely the particle $n+1$ and recover a correlation function $\rho_{n+m(\overline{\mathcal{D}})}$, multiplied by a factor $N - n - m(\overline{\mathcal{D}})$ (see definition (2.20)). This correspond to operation 5 of the list at page 41, and produces the term in the first line of (5.13).

The error term in the preceding extension of the integration region will contain an integral over the states x'_{n+1} of the particle $n+1$ at time zero such that "there exists a *first* collision (in $[0,t]$) with at least one of the particles of the evolutions associated to $\overline{\mathcal{D}}_{0;n+1}$". This integral function is in turn integrated over all such evolutions, that is over all the collision histories $\mathcal{D}'$ that are compatible with the tree $\overline{\mathcal{D}}_{0;n+1}$. Calling $t^*, \hat{p}^*, \hat{w}^*$ the time, momentum and unit vector variables describing, in the usual way, the state of the free evolution of x'_{n+1} *ingoing* its first collision with the particles of $\mathcal{E}_{\mathcal{D}'}$, we can proceed as before by making the change of variables $x'_{n+1} \longrightarrow (t^*, \hat{p}^*, \hat{w}^*)$. Again we have resulting integrals $\int dt^* \int d\hat{p}^* \int_{\Omega^{(*)}_{i-}} d\hat{w}^*$ corresponding to a new node to be added to $\overline{\mathcal{D}}_{0;n+1}$, and a Jacobian determinant producing the associated weight factor. The net effect is the value of a tree produced via operations 1 and 2 of the list at page 41, when the integrations associated to the new node are restricted to "*incoming collisions* producing a particle that *does not collide* with the particles of the evolution for all times in the past from t^* up to 0". This term, together with the one obtained in the above paragraph, gives, once summed over all the possible choices of particle i, the term in the second line of (5.13).

The case $m(\overline{\mathcal{D}}_{0;n+1}) \neq 0$ is treated in the same way, with the only important difference that the role played by time 0 is now played by $t_{l^*(\overline{\mathcal{D}})} \equiv t_{q_1^{(n+1)}(\overline{\mathcal{D}})}$, see Appendix B.2. Here we only mention that, in particular, the "last collision" has to be understood in the time interval $[t_{l^*}, t]$, and in the terms with "no last collision" we perform a change of variable $x_{n+1} \longrightarrow x'_{n+1} = T^{(1)}_{-t+t_{l^*}}(x_{n+1})$. After this change of variables, the extension of the integration region to the whole one particle phase space compatible with the state of the other particles of $\mathcal{E}_{\mathcal{D}}(t_{l^*})$ gives a term that is shown to be identically null, using cancellations between outcoming–incoming collisions occurring at time t_{l^*}. This explains the Kronecker delta in the first line of (5.13).

5.2.3 Second step: cancellations between collision histories

Let us come now to the second step of the proof of Proposition 5.2.1: we will show that we can extend to $\Delta_{\overline{\gamma}_{k,i}}(\underline{x}_n; [0,t])$ the integral in the right hand side of (5.13), since the total contribution of the missing set is equal to zero. This is achieved by the following

Lemma 5.2.1 *In the assumptions of Proposition 5.2.1 and with the notations of (5.12), (5.14), it is*

$$\sum_{k\geq 1}^{l^*} \sum_{i\geq 1}^{n+k-1} \int_{\Delta_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t]) \setminus \Delta^{(*)}_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i} R(\underline{x}_n, \overline{\gamma}_{k,i}, \hat{\gamma}_{k,i}) = 0 \tag{5.15}$$

for almost all $\underline{x}_n \in \Gamma_n$.

Formula (5.15), together with (5.13) and (5.11), complete the proof of Proposition 5.2.1.

We give the proof of the lemma in Appendix C and outline it briefly in the following. Consider the set of all the possible trees of the form $\overline{\mathcal{G}}_{k,i} = (\underline{x}_n, \overline{\gamma}_{k,i}) = \overline{\mathcal{D}}_{/0;n+1} \circ_{k,\underline{q}_+^{(n+1)};i} \overline{\mathcal{D}}_{0;n+1}$, obtained from a given $\overline{\mathcal{D}}$ through the operations 1 – 4 in the list at page 41 (k is the node of $\overline{\mathcal{G}}_{k,i}$ that is created in such operations, and $j_k(\overline{\mathcal{G}}_{k,i}) = i$). In the left hand side of (5.15) we sum and integrate over the corresponding set of collision histories $\mathcal{G}_{k,i}$ such that the associated evolutions satisfy one of the two following special *recollision properties*:

A. the particle generated in the node number k is in outgoing collision at time t_k with particle i and, if we let this particle evolve forward in time together with the particles of the evolution $\mathcal{E}_{\mathcal{G}_{k,i}}(s), s > t_k$, it undergoes a new collision within time t;

B. the particle generated in the node number k is in incoming collision at time t_k with particle i and, in the backwards evolution $\mathcal{E}_{\mathcal{G}_{k,i}}(s), s < t_k$ (of which the particle takes part), it undergoes a new collision within the time of the first node that is found climbing the line generated in node k, or within time 0 if there is no such a node.

We shall refer to the "new collision" as the "recollision" with the other particles of the evolution.

The lemma follows from the observation that for any evolution (i.e. collision history) of type A there is an evolution (collision history) of type B (and viceversa, so that a one by one correspondence is established), giving opposite contribution to the left hand side of (5.15). To find it, *add* to the evolution $\mathcal{E}_{\mathcal{G}_{k,i}}$ of type A the free flow of particle $n+k$ from the time t_k up to the time of the recollision (or, if you start from an evolution of type B, *erase* it from the time of the recollision up to the time t_k). Clearly the new evolution (and associated collision history) that is obtained in this way, say $\mathcal{E}_{\mathcal{G}_{k',i'}}$, is of type B (or A), with k and i substituted by some different values $k' \leq k (\geq k), 1 \leq i' \leq n + k' - 1$. The two evolutions will correspond, in general, to different trees. Moreover, the value of function $R(\mathcal{G}_{k',i'})$ is obtained from $R(\mathcal{G}_{k,i})$ by substitution of the weight factor of node k of $\mathcal{G}_{k,i}$ with the weight factor of node k' of $\mathcal{G}_{k',i'}$. But this is, up to a minus sign, the transformation in the integrand function induced by the change of variables $(t_k, \hat{w}_k) \longrightarrow (t_{k'}, \hat{w}_{k'})$, where $w_k, w_{k'}$ are the unit vectors labelling the nodes k and k' in the two collision histories. Hence the lemma is proved performing this change of variables in the restriction of the integral to the collision histories of type A (or B).

5.3 Sum over trees

Using Proposition 5.2.1, Equation (5.4) becomes

$$\rho_n(\underline{x}_n,t) = \frac{1}{N-n}\Big[\sum_{\substack{\overline{\mathcal{D}}\in\overline{\Delta}(\underline{x}_{n+1};[0,t])\\ m(\overline{\mathcal{D}}_{0;n+1})=0}} \Big(N-n-m(\overline{\mathcal{D}})\Big)\, V(\overline{\mathcal{D}}_{/0;n+1}) + \sum_{\overline{\mathcal{D}}\in\overline{\Delta}(\underline{x}_{n+1};[0,t])} \sum_{k\geq 1}^{l^*} \sum_{i\geq 1}^{n+k-1} V\left(\overline{\mathcal{D}}_{/0;n+1} \circ_{k,\underline{q}_+^{(n+1)};i} \overline{\mathcal{D}}_{0;n+1}\right)\Big] \tag{5.16}$$

for $1 \leq n < N$, a.e. in Γ_n.

The content of the square brackets is graphically represented by a sum of trees of $\overline{\Delta}(\underline{x}_n;[0,t])$ with certain multiplicity factors. Hence, to deduce the assertion of Theorem 4.0.1, we are left with the problem of showing that in this sum we have exactly $N-n$ copies of each tree of $\overline{\Delta}(\underline{x}_n;[0,t])$ – see Figure 5.3 for some example. This follows easily from analysis of the extraction&growth operations described by Proposition 5.2.1, as explained in what follows.

Fix $\overline{\mathcal{G}} \in \overline{\Delta}(\underline{x}_n;[0,t])$, with number of nodes $0 \leq m(\overline{\mathcal{G}}) \leq N-n$. If $m(\overline{\mathcal{G}}) < N-n$, consider the tree $\overline{\mathcal{D}}^{(0)} = \overline{\mathcal{D}}^{(0)}(x_{n+1}) \in \overline{\Delta}(\underline{x}_{n+1};[0,t])$ which is obtained simply adding a coordinate $x_{n+1} \in \Gamma_1(\underline{x}_n)$ (and such that $\underline{x}_{n+1} \in \Gamma^*_{n+1}$) to the root of $\overline{\mathcal{G}}$. It is $m(\overline{\mathcal{D}}^{(0)}_{0;n+1}) = 0$, and we see that $\int_{\Gamma_1(\underline{x}_n)} dx_{n+1}\overline{\mathcal{D}}^{(0)}(x_{n+1})$ produces all the $N-n-m(\overline{\mathcal{G}})$ copies of $\overline{\mathcal{G}}$ that can be obtained through operation 5 in the list at page 41.

Now we want to find all the trees in $\overline{\Delta}(\underline{x}_{n+1};[0,t])$ that produce one or more copies of $\overline{\mathcal{G}}$ via operations 1 – 4 of the list. Suppose that node number k of $\overline{\mathcal{G}}$ is *created* in point 2. Then it is clear that we have one and only one tree producing $\overline{\mathcal{G}}$: this tree can be reconstructed with the following operations:

1'. prune the subtree $\overline{\mathcal{G}}_k$ and delete the node together with the label (if any) attached to it;

2'. reattach the same subtree to $\overline{\mathcal{G}}_{/k}$ in such a way that the root line of $\overline{\mathcal{G}}_k$ is superposed to the root line of $\overline{\mathcal{G}}_{/k}$, and the reciprocal order of the nodes in the resulting tree is the same as it was in $\overline{\mathcal{G}}$;

3'. add a coordinate $x_{n+1} \in \Gamma_1(\underline{x}_n)$ to the root, as well as a label $n+1$ to the new nodes crossed by the root line.

We shall call $\overline{\mathcal{D}}^{(k)} = \overline{\mathcal{D}}^{(k)}(x_{n+1})$ the result of these operations. By construction, we have $\overline{\mathcal{D}}^{(k)} \in \overline{\Delta}(\underline{x}_{n+1};[0,t])$ (for $\underline{x}_{n+1} \in \Gamma^*_{n+1}$), and $\int_{\Gamma_1(\underline{x}_n)} dx_{n+1}\overline{\mathcal{D}}^{(k)}(x_{n+1})$ produces a copy of $\overline{\mathcal{G}}$ when node number k is created in operation 2 of the list at page 41.

The operations 1' – 3' can be repeated for any node of $\overline{\mathcal{G}}$, giving $m(\overline{\mathcal{G}})$ trees (some of which are possibly equivalent) in $\overline{\Delta}(\underline{x}_{n+1};[0,t])$. In particular, we have exactly $m(\overline{\mathcal{G}})$ different ways to produce $\overline{\mathcal{G}}$ through operations 1 – 3, hence operation 4 gives $m(\overline{\mathcal{G}})$ copies of $\overline{\mathcal{G}}$. These copies, together with the previous $N-n-m(\overline{\mathcal{G}})$ copies obtained by operation 5, give the total number of $N-n$ copies of $\overline{\mathcal{G}}$ appearing in the square brackets in (5.16), thus concluding the proof of the Theorem. $\square$

Chapter 6

Comments, comparisons and perspectives

Let us summarize what we have done in the previous chapters. We discussed a derivation of the series expansion used by Lanford [27] to perform the Boltzmann–Grad limit, expressing the time–evolved $n-$points correlation function in terms of the higher order correlation functions at time zero for a system of N hard spheres in a finite volume. We established a new method of construction of the series based on step by step direct integration of degrees of freedom from the solution of Liouville equation, rather than iteration of the BBGKY equations. Each term of the expansion was written in the form of integral over some fictitious evolutions of particles called "collision histories", for which we could introduce a convenient graphical representation. We showed that these graphs can be used to control the integration procedure leading from the expansion for ρ_{n+1} to the expansion for ρ_n. Mutual cancellations between collision histories showing special "recollision properties" were exhibited as an important part of the proof. The method provides a construction of the series expansion in a fixed full measure subset of the phase space, under the only hypothesis of some integrable bound for the density of the initial measure, and symmetry in the particle labels. This strengthens the results previously obtained in literature. We stated also an extension of the main theorem to initial measures with non definite number of particles.

Without assuming continuity along trajectories of the initial measure, we could resum the final expansion and recover the usual BBGKY hierarchy of integro–differential equations for hard spheres, as originally deduced by Cercignani in [6] (and rigorously obtained in [23] by using the continuity assumptions). In fact, the final expansion can be also seen as the series solution of the Cauchy problem for the BBGKY hierarchy: actually this is the way it was presented in [27] where, nevertheless, a rigourous discussion was still missing. In the hard sphere systems, the rigorous analysis of the dynamics and derivation of the BBGKY equations is more complicated than for smooth potentials (which was well known at the time of [27]), because of the singular character of the interaction. Such an analysis was realized, for the Hamiltonian dynamics, in [3] and [32], while the rigorous derivation of the hierarchy was first made by Spohn in [45]. In what follows we make some comparison with that note.

The starting point in [45] is an equation (Proposition 1, formula (20)) expressing the variation $\rho_n(x_1, \cdots, x_n, t) - \rho_n(T^{(n)}_{-t}(x_1, \cdots, x_n))$ as a *sum* over the number of collisions in $[0, t]$ between the cluster of particles $(1, \cdots, n)$ and the others $(n + 1, \cdots, N)$, of the corresponding gain and loss terms expressed through the initial probability measure P. This equation can be considered already as a rough form of the BBGKY hierarchy: the goal is to show that the sum of all the gain and loss terms is absolutely continuous with respect to the Lebesgue measure and has a density given by the collision operator of the hierarchy applied to ρ_{n+1}, i.e. to *compute* the derivative of those terms with respect to the time. To do this, some probability estimate on the number of collisions is needed, together with the continuity along trajectories of the initial measure. After that, the expansion of Lanford is derived, as usual, via iteration of the hierarchy. Finally, it is rephrased as an integral over collision histories and then extended to non continuous measures of grand canonical type by a density argument.

Coming back to the starting point, formula (20), we see that it does not keep track of what the external particles colliding with $(1, \cdots, n)$ do during $[0, t]$, and that a control on the number of collisions in the time interval is required. As we saw, in the notion of collision history every time, going backwards, an external particle collides with $(1, \cdots, n)$, we add it to the cluster $(1, \cdots, n)$ and keep looking at it. We saw also that, using this notion, we can directly express the variation $\rho_n(x_1, \cdots, x_n, t) - \rho_n(T^{(n)}_{-t}(x_1, \cdots, x_n))$ as a sum over the number of *new* particles that can appear in the history, rather than over the number of collisions. In this way, *provided* we introduce the notion of collision history from the beginning, we can construct directly the final expansion (without the need of strong estimates nor continuity assumptions). Notice also that this construction is carried on through nothing but the same kind of steps leading to Eq. (20) of [45]: a decomposition of the phase space, a flow of the coordinates (change of variables) from time t to the time of the last collision or to time zero, cancellations between sets.

There are various other rigorous discussions on the hierarchy and the series expansion for hard spheres. A derivation of the BBGKY hierarchy in the form of integro–differential equations is given in [23]. There the authors show that, using the special flow representation introduced in [32], a weak version of the hierarchy (integrated against test functions in a suitable space) can be derived. The final result follows then from uniqueness of the solution of the weak equations in the case of initial measure continuous along trajectories. Another discussion that has to be mentioned is in the work by K. Uchiyama [47], where the same results of [45] are proved in a similar way, with the continuity along trajectories of the initial data substituted by the continuity over almost every point of the phase space (at the end removed again by density). Finally, other rigorous analysis on the Cauchy problem for the BBGKY hierarchy can be found in the works of D. Ya. Petrina and V. I. Gerasimenko, see [19], [36] or the book [37].

We hope that the methods presented in the previous chapters can be used to deal with different situations. For instance, we believe that the whole analysis can be applied to discrete initial measures. Another direction of research would be the derivation of the smooth potentials case: following the ideas of [24] the procedure valid for the hard sphere case can be probably extended. Finally, it would be interesting to apply our methods to the construction of the series expansions in cases with boundary conditions different from those used here, and suitable for modeling of open systems.

Chapter 7

Constructive integration of the BBGKY

In this chapter we deal with the problem of establishing a constructive iterative integration method for the infinite BBGKY hierarchy, in the equilibrium setting and for smooth interactions. In Section 7.1 we setup the problem and give the definitions needed. In Section 7.2 we present a new method of integration directly leading to the Kirkwood–Salsburg equations. In Section 7.3 we discuss an alternative procedure inspired by paper [17], and make comparisons with it.

7.1 The infinite system of particles

We will concern with an infinite classical system of particles interacting through a smooth positive pair potential with finite range. We will introduce a class of measures over the phase space of the system, with properties that assure the existence of smooth correlations, and the infinite hierarchy of equations satisfied by them. We list below the definitions required.

1) The *phase space* $\mathcal{H}$ is given by the infinite countable sets $X = \{x_i\}_{i=0}^{\infty} \equiv \{(q_i, p_i)\}_{i=0}^{\infty}$, $x_i \in \mathbb{R}^\nu \times \mathbb{R}^\nu, \nu = 1, 2, 3$, which are locally finite: $\Lambda \cap (\cup_{i=0}^{\infty} q_i)$ is finite for any bounded region $\Lambda \subset \mathbb{R}^\nu$.

2) The *Hamiltonian* of the system is defined by the formal function on $\mathcal{H}$

$$H(X) = \sum_{i=1}^{\infty} \frac{p_i^2}{2} + \sum_{i<j}^{0,\infty} \varphi(q_i - q_j) \ , \tag{7.1}$$

where $\varphi : \mathbb{R}^\nu \to \mathbb{R}^+$ is assumed to be a C^1 positive function with compact support, depending only on $|q|$.

3) A *state* is a probability measure μ on the Borel sets of $\mathcal{H}$ (see [41], [40]). Following [40], we may define it as a collection $\{\mu_\Lambda\}$ of probability measures on $\mathcal{H}_\Lambda := \oplus_{n=0}^{\infty}(\Lambda \times \mathbb{R}^\nu)^n$, $\Lambda \subset \mathbb{R}^\nu$ bounded open, satisfying the following properties:

a. the restriction of μ_Λ on the space $(\Lambda \times \mathbb{R}^\nu)^n$ is absolutely continuous with respect to Lebesgue measure, with a density of the form $\frac{1}{n!}\mu_\Lambda^{(n)}(x_1, \cdots, x_n)$, symmetric for exchange of particles;

b. $\mu_\emptyset^0(\mathbb{R}^0 \times \mathbb{R}^0) = 1$;

c. if $\Lambda \subset \Lambda'$, then

$$\mu_\Lambda^{(n)}(x_1, \cdots, x_n) = \sum_{p=0}^{\infty} \frac{1}{p!} \int_{((\Lambda' \backslash \Lambda) \times \mathbb{R}^\nu)^p} dx_{n+1} \cdots dx_{n+p} \mu_{\Lambda'}^{(n+p)}(x_1, \cdots, x_{n+p}) \; ; \tag{7.2}$$

d. $\mu_\Lambda^{(n)} \leq C_\Lambda^n \prod_{i=1}^n \eta_\Lambda(|p_i|)$ for some constant C_Λ and $\eta_\Lambda(|p|) \in L^1(\mathbb{R}^\nu)$, so that the expression in the right hand side of the following equation is well defined:

$$\overline{\rho}_n(x_1, \cdots, x_n) := \sum_{p=0}^{\infty} \frac{1}{p!} \int_{(\Lambda \times \mathbb{R}^\nu)^p} dx_{n+1} \cdots dx_{n+p} \mu_\Lambda^{(n+p)}(x_1, \cdots, x_{n+p}) \; , \tag{7.3}$$

where we assume $q_1, \cdots, q_n \in \Lambda$;

e. there exist $\xi > 0, \eta(|p|) \in L^1(\mathbb{R}^\nu), |p|\eta(|p|) \in L^1(\mathbb{R}^\nu)$, such that

$$\overline{\rho}_n(x_1, \cdots, x_n) \leq \xi^n \prod_{i=1}^n \eta(|p_i|) \; . \tag{7.4}$$

Equation (7.3) defines the *correlation functions* of the state.

The state is said to be *smooth* if its correlation functions are C^1 functions on $(\mathbb{R}^\nu \times \mathbb{R}^\nu)^n$ with derivative bounded by $|\frac{\partial \overline{\rho}_n}{\partial x_i}| \leq C_n \xi^n \prod_{j=1}^n \eta(|p_j|)$, for some $C_n > 0$. It is said to be *invariant* if

$$\mu_\Lambda^{(n)}(x_1, \cdots, x_n) = \mu_{\Lambda+a}^{(n)}(q_1 + a, p_1, \cdots, q_n + a, p_n) \tag{7.5}$$

for all $a \in \mathbb{R}^\nu$ and Λ.

Remarks. (i) Condition **b.**, together with the compatibility condition **c.**, imply the normalization of the measures μ_Λ, i.e.

$$\sum_{n \geq 0} \frac{1}{n!} \int_{(\Lambda \times \mathbb{R}^\nu)^n} dx_1 \cdots dx_n \mu_\Lambda^{(n)}(x_1, \cdots, x_n) = 1 \; . \tag{7.6}$$

(ii) Condition **e.** guarantees convergence of the inverse formula

$$\mu_\Lambda^{(n)}(x_1, \cdots, x_n) = \sum_{p=0}^{\infty} \frac{(-1)^p}{p!} \int_{(\Lambda \times \mathbb{R}^\nu)^p} dx_{n+1} \cdots dx_{n+p} \overline{\rho}_{n+p}(x_1, \cdots, x_{n+p}) \; ; \tag{7.7}$$

hence the definition of correlation functions of the state is well posed. (iii) The definition (7.3) implies that an invariant state has also translation invariant correlation functions.

Finally, a state is *Maxwellian* when there exist $\rho_n : \mathbb{R}^{\nu n} \to \mathbb{R}^+$ such that the correlation functions have the form

$$\overline{\rho}_n(x_1, \cdots, x_n) = \prod_{i=1}^{n} \left(\frac{e^{-\beta p_i^2/2}}{(2\pi/\beta)^\nu} \right) \rho_n(q_1, \cdots, q_n) , \qquad \beta > 0 . \tag{7.8}$$

4) A smooth state is a *stationary solution* of the *BBGKY hierarchy* of equations with Hamiltonian H if

$$\begin{aligned}
&\sum_{i=1}^{n} [p_i \cdot \nabla_{q_i} \overline{\rho}_n(x_1, \cdots, x_n) - \nabla_{q_i} W_{q_i}(q_1, \cdots q_{i-1}, q_{i+1}, \cdots, q_n) \cdot \nabla_{p_i} \overline{\rho}_n(x_1, \cdots, x_n)] \\
&\quad = \sum_{i=1}^{n} \int_{\mathbb{R}^\nu \times \mathbb{R}^\nu} d\xi d\pi \nabla_{q_i} \varphi(q_i - \xi) \cdot \nabla_{p_i} \overline{\rho}_{n+1}(x_1, \cdots, x_n, \xi, \pi) , \qquad n \geq 1 ,
\end{aligned} \tag{7.9}$$

for any $(x_1, \cdots, x_n) \in \mathbb{R}^{2\nu n}$, where

$$W_q(q_1, \cdots, q_n) = \sum_{i=1}^{n} \varphi(q - q_i) . \tag{7.10}$$

Remarks. (i) The solutions to the Newton equations of the infinite system of particles with Hamiltonian H can be constructed in any dimension for a large class of potentials in a full set of initial data in $\mathcal{H}$, with respect to a Gibbs measure; see for instance [31] and [27]. The result has been also extended in several cases to much larger classes of (nonequilibrium) measures, e.g. [25], [26] (for $\nu = 1$), [13] (for $\nu = 2$) and [8] (for $\nu = 3$). (ii) In all these cases the time evolution of a state is generally described, at least for smooth correlations, by the BBGKY hierarchy of equations ([9]), that is Equation (7.9) for time dependent correlation functions and with the additional term $\frac{\partial}{\partial t} \overline{\rho}_n(x_1, \cdots, x_n, t)$ in the left hand side.

7.2 Integration of the equilibrium hierarchy

We want to solve Equation (7.9), after having assumed that the state is invariant and Maxwellian with parameter $\beta > 0$, [33]. Thus the problem is equivalent to consider the following infinite system:

$$\begin{aligned}
\nabla_{q_1} \rho_n(q_1, \cdots, q_n) = -\beta \Big[&\nabla_{q_1} W_{q_1}(q_2, \cdots, q_n) \rho_n(q_1, \cdots, q_n) \\
&+ \int_{\mathbb{R}^\nu} dy \nabla_{q_1} \varphi(q_1 - y) \rho_{n+1}(q_1, \cdots, q_n, y) \Big] , \qquad n \geq 1 ,
\end{aligned} \tag{7.11}$$

for $\rho_n \in C^1(\mathbb{R}^{\nu n})$ symmetric in the exchange of particle labels, translation invariant and bounded as

$$\rho_n \leq \xi^n \;, \qquad \xi > 0 \;, \tag{7.12}$$

with

$$|\nabla_{q_i}\rho_n| \leq C_n \xi^n \;, \qquad C_n > 0, i = 1, \cdots, n \;. \tag{7.13}$$

The equations are then parametrized by the two positive constants $\rho \equiv \rho_1(q_1)$, and $\beta > 0$. The Eq. (7.11) for $n = 1$ will be useless in our assumptions.

To achieve the integration we need to add some boundary condition. We choose the *cluster property* defined as follows. Denote A_n and B_m any two disjoint clusters of n and m points respectively in $\mathbb{R}^\nu$, such that $A_n \cup B_m = (q_1, \cdots, q_{n+m})$. Indicate $\mathrm{dist}(A_n, B_m) = \inf\{|q_i - q_j|; q_i \in A_n, q_j \in B_m\}$. Then there exists a constant $C > 0$ and a monotonous decreasing function u vanishing at infinity such that

$$|\rho_{n+m}(A_n, B_m) - \rho_n(A_n)\rho_m(B_m)| \leq C^{n+m} u(\mathrm{dist}(A_n, B_m)) \;. \tag{7.14}$$

This is known to be satisfied by every equilibrium state at least for sufficiently small density (small ρ) or high temperature (small β); [39].

Our main result is the following

Theorem 7.2.1 *If a smooth Maxwellian invariant state is a stationary solution of the BBGKY hierarchy with cluster boundary conditions, then there exists a constant z such that the correlation functions of the state satisfy*

$$\begin{aligned} \rho_n(q_1, \cdots, q_n) = z e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \Big[& \rho_{n-1}(q_2, \cdots, q_n) \\ & + \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \int_{\mathbb{R}^{m\nu}} dy_1 \cdots dy_m \\ & \cdot \prod_{j=1}^{m} \left(1 - e^{-\beta\varphi(q_1 - y_j)}\right) \rho_{n-1+m}(q_2, \cdots, q_n, y_1, \cdots, y_m) \Big] \;. \end{aligned} \tag{7.15}$$

Conversely, a smooth Maxwellian state satisfying (7.15) is a stationary solution of the BBGKY hierarchy.

The integral relations (7.15) are called the *Kirkwood–Salsburg equations.* The series in the right hand side is absolutely convergent uniformly in $q_1, \cdots, q_n$ since φ has compact support and $\rho_n \leq \xi^n$. We shall point out that, for $n = 1$, the first term in the right hand side has to be interpreted as z; the Equation is in this case independent of q_1 by translation invariance: it provides a definition of z in terms of integrals of all the correlation functions. Formula (7.15) is one of the several characterizations of an *equilibrium* state, and z is identified with the *activity* of the system, e.g. [30], [42], [12], [22].

Proof of Theorem 7.2.1. We prove here the direct statement. The proof of the converse statement is analogous to the one of point *(iii)* in Proposition 8.0.1, which will be discussed in Chapter 8.

In primis, we rewrite (7.11) as

$$e^{\beta W_{q_1}(q_2,\cdots,q_n)}\Big(\nabla_{q_1}\rho_n(q_1,\cdots,q_n)+\beta\rho_n(q_1,\cdots,q_n)\nabla_{q_1}W_{q_1}(q_2,\cdots,q_n)\Big)$$
$$=-\beta\int_{\mathbb{R}^3}dy\nabla_{q_1}\varphi(q_1-y)e^{\beta W_{q_1}(q_2,\cdots,q_n)}\rho_{n+1}(q_1,\cdots,q_n,y)\ , \tag{7.16}$$

so that the left hand side is equal to $\nabla_{q_1}\left(\rho_n e^{\beta W_{q_1}}\right)$. For the sake of clearness, hereafter we will put

$$\hat\rho_n(q_1;q_2,\ldots,q_n):=e^{\beta W_{q_1}(q_2,\ldots,q_n)}\rho_n(q_1,\ldots,q_n)\ ; \tag{7.17}$$
$$K_{q_0q_1}(q,y):=(1-e^{-\beta\varphi(q-y)})-(1-e^{-\beta\varphi(q_1-y)})-(1-e^{-\beta\varphi(q_0-y)})\ .$$

The $\hat\rho_n$ satisfy

$$\nabla_{q_1}\hat\rho_n(q_1;q_2,\ldots,q_n) \tag{7.18}$$
$$=-\int_{\mathbb{R}^\nu}dy_1\nabla_{q_1}\left(1-e^{-\beta\varphi(q_1-y_1)}\right)\hat\rho_{n+1}(q_1;q_2,\ldots,q_n,y_1)\ .$$

Fix $q_0\in\mathbb{R}^\nu$ arbitrarily. We shall integrate the previous equation along a straight line $\overrightarrow{q_0q_1}$ connecting q_0 to q_1. Using the smoothness assumption and (7.17) we deduce

$$\hat\rho_n(q_1;q_2,\ldots,q_n)-\hat\rho_n(q_0;q_2,\ldots,q_n) \tag{7.19}$$
$$=-\int_{q_0}^{q_1}d\bar q_1\int_{\mathbb{R}^d}dy_1\frac{\partial K_{q_0q_1}}{\partial\bar q_1}(\bar q_1,y_1)\hat\rho_{n+1}(\bar q_1;q_2,\ldots,q_n,y_1)\ ,$$

where $\int_{q_0}^{q_1}d\bar q_1$ and $\frac{\partial}{\partial\bar q_1}$ denote respectively integration and differentiation along the straight line. Interchanging the integrations in the right hand side and integrating by parts we find

$$\hat\rho_n(q_1;q_2,\ldots,q_n)-\hat\rho_n(q_0;q_2,\ldots,q_n) \tag{7.20}$$
$$=-\int dy_1\Big[-\left(1-e^{-\beta\varphi(q_0-y_1)}\right)\hat\rho_{n+1}(q_1;q_2,\ldots,q_n,y_1)$$
$$+\left(1-e^{-\beta\varphi(q_1-y_1)}\right)\hat\rho_{n+1}(q_0;q_2,\ldots,q_n,y_1)\Big]$$
$$+\int_{\mathbb{R}^d}dy_1\int_{q_0}^{q_1}d\bar q_1K_{q_0q_1}(\bar q_1,y_1)\frac{\partial\hat\rho_{n+1}}{\partial\bar q_1}(\bar q_1;q_2,\ldots,q_n,y_1)\ .$$

All the above integrals are absolutely convergent thanks to (7.12), (7.13), smoothness of the potential and compactness of its support.

In the last term of the above equation we may iterate the projection of (7.18) along $\overrightarrow{q_0q_1}$, that can be written as

$$\frac{\partial\hat\rho_n(\bar q_1;q_2,\ldots,q_n)}{\partial\bar q_1}=-\int_{\mathbb{R}^d}dy_1\frac{\partial K_{q_0q_1}}{\partial\bar q_1}(\bar q_1,y_1)\hat\rho_{n+1}(\bar q_1;q_2,\ldots,q_n,y_1)\ . \tag{7.21}$$

The last term of (7.20) then becomes, proceeding as after (7.19),

$$
\begin{aligned}
&-\int_{\mathbb{R}^d} dy_1 \int_{\mathbb{R}^d} dy_2 \int_{q_0}^{q_1} d\bar{q}_1 K_{q_0q_1}(\bar{q}_1, y_1) \\
&\qquad \cdot \frac{\partial K_{q_0q_1}}{\partial \bar{q}_1}(\bar{q}_1, y_2)\hat{\rho}_{n+2}(\bar{q}_1; q_2, \cdots, q_n, y_1, y_2) \\
&= -\frac{1}{2}\int_{\mathbb{R}^d} dy_1 \int_{\mathbb{R}^d} dy_2 \Big[\prod_{j=1,2} \left(1 - e^{-\beta\varphi(q_0-y_j)}\right) \hat{\rho}_{n+2}(q_1; q_2, \ldots, q_n, y_1, y_2) \\
&\qquad + \prod_{j=1,2} \left(1 - e^{-\beta\varphi(q_1-y_j)}\right) \hat{\rho}_{n+2}(q_0; q_2, \ldots, q_n, y_1, y_2)\Big] \\
&+\frac{1}{2}\int_{\mathbb{R}^d} dy_1 \int_{\mathbb{R}^d} dy_2 \int_{q_0}^{q_1} d\bar{q}_1 \prod_{j=1,2} K_{q_0q_1}(\bar{q}_1, y_j) \frac{\partial \hat{\rho}_{n+2}}{\partial \bar{q}_1}(\bar{q}_1; q_2, \ldots, q_n, y_1, y_2)\ ,
\end{aligned}
\tag{7.22}
$$

having used also the symmetry for exchange of particles to perform the integration by parts. We may iterate again (7.21) in the last term of this formula. After $N-1$ iterations (N integrations by parts) we have

$$
\begin{aligned}
&\hat{\rho}_n(q_1; q_2, \ldots, q_n) - \hat{\rho}_n(q_0; q_2, \ldots, q_n) \\
&= -\sum_{k=1}^{N} \frac{(-1)^k}{k!} \int dy_1 \cdots dy_k \Big[\prod_{j=1}^{k} \left(1 - e^{-\beta\varphi(q_0-y_j)}\right) \hat{\rho}_{n+k}(q_1; q_2, \cdots, q_n, y_1, \cdots, y_k) \\
&\qquad - \prod_{j=1}^{k} \left(1 - e^{-\beta\varphi(q_1-y_j)}\right) \hat{\rho}_{n+k}(q_0; q_2, \cdots, q_n, y_1, \cdots, y_k)\Big] \\
&\quad -\frac{1}{N!}\int dy_1 \cdots dy_{N+1} \int_{q_0}^{q_1} d\bar{q}_1 \prod_{j=1}^{N} K_{q_0q_1}(\bar{q}_1, y_j) \\
&\qquad \cdot \frac{\partial K_{q_0q_1}}{\partial \bar{q}_1}(\bar{q}_1, y_{N+1}) \hat{\rho}_{n+N+1}(\bar{q}_1; q_2, \cdots, q_n, y_1, \cdots, y_{N+1})\ .
\end{aligned}
\tag{7.23}
$$

Call $\overline{\varphi}$ the maximum value of φ. The assumptions on the interaction potential and (7.12) allow to bound explicitly the last term with

$$
\begin{aligned}
&\frac{1}{N!}|q_1 - q_0| \left(3\int_{\mathbb{R}^\nu} dy \left(1 - e^{-\beta\varphi(y)}\right)\right)^N \\
&\qquad \cdot \left(\int_{\mathbb{R}^\nu} dy |\nabla(1 - e^{-\beta\varphi(y)})|\right) \left(e^{\beta\overline{\varphi}}\right)^{n+N} \xi^{n+1+N}\ .
\end{aligned}
\tag{7.24}
$$

Thus by taking $N \to \infty$, it follows that, for any arbitrary $q_0 \in \mathbb{R}^\nu$, the correlation functions satisfy the set of integral equations

$$
\begin{aligned}
&e^{-\beta W_{q_0}(q_2, \cdots, q_n)} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int dy_1 \cdots dy_k \prod_{j=1}^{k} \left(1 - e^{-\beta\varphi(q_0-y_j)}\right) \\
&\quad \cdot e^{\beta W_{q_1}(y_1, \cdots, y_k)} \rho_{n+k}(q_1, q_2, \cdots, q_n, y_1, \cdots, y_k) \\
&= e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int dy_1 \cdots dy_k \prod_{j=1}^{k} \left(1 - e^{-\beta\varphi(q_1-y_j)}\right) \\
&\quad \cdot e^{\beta W_{q_0}(y_1, \cdots, y_k)} \rho_{n+k}(q_0, q_2, \cdots, q_n, y_1, \cdots, y_k)\ ,
\end{aligned}
\tag{7.25}
$$

where the series in both sides are absolutely convergent uniformly in $q_0, q_1, \cdots, q_n$. Notice that the exponentials $e^{\beta W_{q_1}(y_1,\cdots,y_k)}$ and $e^{\beta W_{q_0}(y_1,\cdots,y_k)}$ disappear from the formula as soon as $|q_1 - q_0|$ is greater than twice the range of the potential.

What is left in order to complete the proof is just taking the limit as $|q_0| \to \infty$ of (7.25). Here we need the invariance assumption and the cluster property (7.14) which, together with finiteness of the range of the integrand, imply

$$\rho_n(q_1,\cdots,q_n)\Big[1+\sum_{k=1}^{\infty}\frac{(-1)^k}{k!}\int dy_1\cdots dy_k \prod_{j=1}^{k}\Big(1-e^{-\beta\varphi(y_j)}\Big)\rho_k(y_1,\cdots,y_k)\Big]$$
$$= \rho e^{-\beta W_{q_1}(q_2,\cdots,q_n)}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\int dy_1\cdots dy_k$$
$$\cdot\prod_{j=1}^{k}\Big(1-e^{-\beta\varphi(q_1-y_j)}\Big)\rho_{n-1+k}(q_2,\cdots,q_n,y_1,\cdots,y_k)\ . \tag{7.26}$$

The factor in the square brackets on the left hand side is a strictly positive constant depending on β and $\rho_k, k \geq 1$; this follows by using that ρ_k are correlation functions of a probability measure, and it is checked for completeness in Appendix E. The direct statement of the Theorem is thus proved by calling

$$z = \frac{\rho}{\Big[1+\sum_{k=1}^{\infty}\frac{(-1)^k}{k!}\int dy_1\cdots dy_k\prod_{j=1}^{k}\Big(1-e^{-\beta\varphi(y_j)}\Big)\rho_k(y_1,\cdots,y_k)\Big]}\ . \tag{7.27}$$

□

Clearly, the direct statement has no meaning for *all* values of the parameters ρ, β, since it could happen that, for given values of those parameters, there are no solutions to the Kirkwood–Salsburg equations obeying the hypothesis of the Theorem. In particular, we refer to translation invariance and cluster properties, which are only proved to be valid inside the “gas phase region” (small ρ / small β). We want to stress also that, outside that region, there could be multiple–valued solutions to Eq. (7.15), including both gaseous and liquid states. Existence and uniqueness are assured by the Theorem just for ξ small, as explained by the next corollary. In any case, we believe that it is interesting for the method to work for any value of ξ, unlike the one presented in [17], and like that of [33]. Moreover, the dependence on the free parameter q_0 of formula (7.25) (which has been derived without using the translation invariance or the cluster property) can be used to take into account even different boundary conditions and/or symmetry assumptions; for instance we will see in the next section the case of an equilibrium system in an infinite container.

Corollary 7.2.1 *In the hypothesis of the Theorem, for ξ sufficiently small the state is uniquely determined by ρ, β, and it coincides with the (unique) solution of (7.15).*

Proof of Corollary 7.2.1. The result follows from the well known theory of convergence of the Mayer expansion for z small [38], [34], after noting from Eq. (7.27) that $z = O(\xi)$ for ξ small. We sketch the proof for completeness.

By iteration of (7.15) we get the formal expansions

$$\rho = z\sum_{p=0}^{\infty} c_{1,p} z^p$$

$$\rho_n(q_1, \cdots, q_n) = z\sum_{p=0}^{\infty} c_{n,p}(q_1, \cdots, q_n) z^p \ , \qquad n > 1 \ , \tag{7.28}$$

where the coefficients are defined in terms of β and φ by the explicit recursive relation

$$\begin{aligned} & c_{n,0} = \delta_{n,1} \qquad\qquad (7.29)\\ & c_{n,p+1}(q_1, \cdots, q_n) = e^{-\beta \sum_{j=2}^{n} \varphi(q_1 - q_j)} \Big[\delta_{n>1} c_{n-1,p}(q_2, \cdots, q_n) \\ & \quad + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int dy_1 \cdots dy_k \\ & \qquad \cdot \prod_{j=1}^{k} \Big(1 - e^{-\beta\varphi(q_1 - y_j)}\Big) c_{n+k-1,p}(q_2, \cdots, q_n, y_1, \cdots, y_k) \Big] \ , \qquad p \geq 0 \ . \end{aligned}$$

In particular, it follows that

$$c_{n,n-1}(q_1, \cdots, q_n) = e^{-\beta \sum_{i<j}^{0,n} \varphi(q_i - q_j)}$$

and

$$c_{n,p}(q_1, \cdots, q_n) = 0 \text{ for } p < n-1.$$

Calling

$$I_\beta = \int_{\mathbb{R}^\nu} \Big(1 - e^{-\beta\varphi(x)}\Big) \, dx \ , \tag{7.30}$$

by induction on p and using the positivity of the potential one finds the following estimate uniform in $q_1, \cdots, q_n \in \mathbb{R}^\nu$:

$$|c_{n,p}(q_1, \cdots, q_n)| \leq I_\beta^{-(n-1)} (I_\beta e)^p \ . \tag{7.31}$$

Hence the expansions (7.28) are absolutely convergent uniformly in the coordinates, as soon as

$$|z| < (eI_\beta)^{-1} \ . \tag{7.32}$$

The first equation ($n = 1$) is, in this case, the expansion of ρ in powers of z, an it is of the form $\rho = z + O(z^2)$: thus it can be inverted for z small, to determine z as a function of ρ and β.

Therefore, to obtain the corollary it is sufficient to take

$$\xi < (2eI_\beta)^{-1} \, . \tag{7.33}$$

In fact, with this choice the denominator in (7.27) is bounded from below by $1 - I_\beta \xi e^{I_\beta \xi} > 1/2$, so that $|z| \leq 2\xi$ and Eq. (7.32) is satisfied. □

7.2.1 Infinite containers

The proof of Theorem 7.2.1 can be easily adapted to cover the more general case of a non invariant state for which translation invariance holds just as a "boundary condition at infinity" in dimensions 2 and 3. We discuss this in the present section. Here we will call r_0 the range of φ, that is $r_0 = \inf\{r \text{ s.t. } \varphi(q) = 0 \text{ for } |q| > r\}$. Consider an open unbounded set $\Lambda_\infty \subset \mathbb{R}^\nu$ with the following properties:

(a) Λ_∞ is polygonally connected;

(b) for any $q \in \Lambda_\infty$, there exists a polygonal path $\Gamma(q)$ connecting q to ∞ such that

$$\text{dist}(\partial\Lambda_\infty, \{y \in \Gamma(q) \text{ s.t. } |y| > n\}) > r_0 \tag{7.34}$$

for sufficiently large n (here dist is the usual distance between sets in $\mathbb{R}^\nu$).
This includes all reasonable geometries suitable for the modeling of a very large container of particles.

The associated phase space, denoted $\mathcal{H}_{\Lambda_\infty}$, is defined as in point 1) of Section 7.1 with the q_i restricted to Λ_∞. All the other definitions of Section 7.1 are extended as well to the system on Λ_∞, just by restricting the coordinates $q_i \in \Lambda_\infty$. In particular, a smooth Maxwellian state on $\mathcal{H}_{\Lambda_\infty}$ is a collection of probability measures on $\mathcal{H}_\Lambda$ with $\Lambda \subset \Lambda_\infty$ bounded open, satisfying properties **a.–e.** of Section 7.1, with correlation functions of the form (7.8),

$$\rho_n \in C^1(\Lambda_\infty) \bigcap C(\overline{\Lambda}_\infty) \tag{7.35}$$

and satisfying also estimates (7.12) and (7.13) over Λ_∞.

The stationary BBGKY hierarchy of equations for such a state reduces to

$$\begin{aligned} \nabla_{q_1} \rho_n(q_1, \cdots, q_n) = -\beta \Big[& \nabla_{q_1} W_{q_1}(q_2, \cdots, q_n) \rho_n(q_1, \cdots, q_n) \\ & + \int_{\Lambda_\infty} dy \nabla_{q_1} \varphi(q_1 - y) \rho_{n+1}(q_1, \cdots, q_n, y) \Big] \, , \qquad n \geq 1 \, , \end{aligned} \tag{7.36}$$

for $q_1, \cdots, q_n \in \Lambda_\infty$, which we shall integrate with the boundary conditions:

(i) ρ_n satisfy the cluster property (7.14) on Λ_∞;

(ii) ρ_n satisfy the following property which we call *invariance at infinity*: there exists a sequence of translation invariant functions $\{f_n\}_{n=1}^{\infty}, f_n : \mathbb{R}^{\nu n} \to \mathbb{R}^+$, a constant $\tilde{C} > 0$, and two monotonous decreasing functions $\tilde{u}(\cdot), \varepsilon(\cdot)$ vanishing respectively at infinity and at r_0, such that

$$\begin{aligned}|\rho_n(q_0+q_1, q_0+q_2, \cdots, q_0+q_n) - f_n(q_1, q_2, \cdots, q_n)| \\ \leq \tilde{C}^n\left[\tilde{u}(|q_0|) + \varepsilon\left(\mathrm{dist}(\partial\Lambda_\infty, \{q_0+q_1, \cdots, q_0+q_n\})\right)\right]\end{aligned} \tag{7.37}$$

for all $q_0, q_1, \cdots, q_n$ with $q_0+q_1, \cdots, q_0+q_n \in \Lambda_\infty$.

In this section we will call $\rho \equiv f_1(q_1)$. The following extension of Theorem 7.2.1 holds:

Theorem 7.2.2 *If a smooth Maxwellian state on $\mathcal{H}_{\Lambda_\infty}$ is a stationary solution of the BBGKY hierarchy satisfying cluster boundary conditions and invariance at infinity, then there exists a constant z such that*

$$\begin{aligned}\rho_n(q_1, \cdots, q_n) = z e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \Big[\rho_{n-1}(q_2, \cdots, q_n) \\ + \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \int_{\Lambda_\infty^m} dy_1 \cdots dy_m \\ \cdot \prod_{j=1}^{m} \left(1 - e^{-\beta\varphi(q_1 - y_j)}\right) \rho_{n-1+m}(q_2, \cdots, q_n, y_1, \cdots, y_m)\Big] .\end{aligned} \tag{7.38}$$

Conversely, a smooth Maxwellian state on Λ_∞ satisfying (7.38) is a stationary solution of the BBGKY hierarchy.

These are the Kirkwood–Salsburg equations in the infinite container. For $n = 1$ the first term in the right hand side has to be interpreted as z. In this case the equation is not independent on q_1 : a definition of z in terms of explicitely constant functions follows using (7.37), by sending q_1 to infinity, keeping it well inside Λ_∞ (that is at least at a distance r_0 from the boundary $\partial\Lambda_\infty$), which is certainly possible in our assumption *(b)* on the geometry of the container (see Eq. (7.40) below).

Proof of Theorem 7.2.2. All that is said in the proof of Theorem 7.2.1 up to the formula (7.25) can be repeated here by restricting the coordinates to Λ_∞, substituting the integration region $\mathbb{R}^\nu$ with Λ_∞, and the straight line $\overrightarrow{q_0 q_1}$ with a polygonal path entirely contained in Λ_∞ connecting q_0 to q_1. We obtain that Eq. (7.25) is valid with $q_0 \in \Lambda_\infty$ and the integrals restricted to Λ_∞^k. Take the limit of this expression as $|q_0| \to \infty$ with q_0 moving along a path $\Gamma(q_1)$ defined as in point *(b)* above: properties *(i)* and *(ii)* and the finiteness of the range of φ imply

$$\rho_n(q_1, \cdots, q_n)\Big[1 + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_{\mathbb{R}^{\nu k}} dy_1 \cdots dy_k \prod_{j=1}^{k} \Big(1 - e^{-\beta\varphi(y_j)}\Big) f_k(y_1, \cdots, y_k)\Big]$$

$$= \rho e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{\Lambda_\infty^k} dy_1 \cdots dy_k$$

$$\cdot \prod_{j=1}^{k} \Big(1 - e^{-\beta\varphi(q_1 - y_j)}\Big) \rho_{n-1+k}(q_2, \cdots, q_n, y_1, \cdots, y_k) \; . \tag{7.39}$$

The factor in the square brackets on the left hand side is a strictly positive constant depending on β and $f_k, k \geq 1$ (apply the discussion in Appendix E). The direct statement of the Theorem is thus proved by calling

$$z = \frac{\rho}{\Big[1 + \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_{\mathbb{R}^{\nu k}} dy_1 \cdots dy_k \prod_{j=1}^{k} \Big(1 - e^{-\beta\varphi(y_j)}\Big) f_k(y_1, \cdots, y_k)\Big]} \; . \tag{7.40}$$

$\square$

The proof of Corollary 7.2.1 can be also adapted to the present case in an obvious way. Relations (7.28)–(7.29) with $\rho, c_{1,p}$ replaced by $\rho_1(q_1), c_{1,p}(q_1)$ and all the involved coordinates restricted to Λ_∞, show that if ξ is taken as in (7.33), Equations (7.38) have a unique solution determined by $\rho = f_1$ and β, and compatible with the assumptions of Theorem 7.2.2. In particular, this solution is actually translation invariant in the region $\{q_1, \cdots, q_n \in \Lambda_\infty, \mathrm{dist}(\partial\Lambda_\infty, q_i) > r_0\}$, as follows by induction on p from Eq. (7.28). The activity z is given in this case by the inversion of the power series

$$\rho = z \sum_{p=0}^{\infty} \left(\lim_{\substack{|q| \to \infty \\ \mathrm{dist}(\partial\Lambda_\infty, q) > r_0}} c_{1,p}(q) \right) z^p \; , \tag{7.41}$$

where the coefficients of the expansion are independent on the way the limit is taken.

Corollary 7.2.2 *In the hypothesis of Theorem 7.2.2, for ξ sufficiently small the state is uniquely determined by ρ, β, and it coincides with the (unique) solution of (7.15).* $\square$

7.3 The method of [17]

In this chapter we discuss the method established in [17] for the integration of the hierarchy (7.11). We point out an error in the formula for the activity. We modify the proof in order to obtain a correct expression, leaving essentially unchanged the procedure.

We will need somewhat stronger assumptions than those of Theorem 7.2.1, namely the smooth state is Maxwellian with positional correlation functions ρ_n satisfying:

a) $\rho_n(q_1, \cdots, q_n) \leq \xi^n$, with ξ small enough;

b) ρ_n are translation and rotation invariant;

c) ρ_n satisfy an exponential strong cluster property, i.e.

$$|\rho_n^T(q_1, \cdots, q_n)| \leq (C\xi)^n e^{-\kappa|q_1 - q_n|} , \qquad C, \kappa > 0 , \tag{7.42}$$

where the *truncated correlation functions* ρ_n^T can be defined by

$$\begin{cases} \rho_2^T(q_1, q_2) = \rho_2(q_1, q_2) - \rho(q_1)\rho(q_2) , \\ \rho_3^T(q_1, q_2, q_3) = \rho_3(q_1, q_2, q_3) - \rho_2(q_1, q_2)\rho(q_3) - \rho(q_1)\rho_2(q_2, q_3) + \rho(q_1)\rho(q_2)\rho(q_3) , \end{cases}$$

etcetera ([11] and [17], page 279).

Let us start by integrating Eq. (7.11) along a straight line connecting q_0 (arbitrary) to q_1 : using the same notations introduced for (7.19), we have

$$\begin{aligned} \rho_n(q_1, \cdots, q_n) &= e^{-\beta\left(W_{q_1}(q_2, \cdots, q_n) - W_{q_0}(q_2, \cdots, q_n)\right)} \rho_n(q_0, q_2, \cdots, q_n) \\ &+ \int_{q_0}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial \bar{q}_1} e^{-\beta\left(W_{q_1}(q_2, \cdots, q_n) - W_{\bar{q}_1}(q_2, \cdots, q_n)\right)} \\ &\cdot \rho_{n+1}(\bar{q}_1, q_2, \cdots, q_n, y_1) . \end{aligned} \tag{7.43}$$

which is nothing but a rewriting of Eq. (7.19). In the assumption *b)*, the case $n = 1$ is a trivial identity, hence we shall assume $n \geq 2$ in the following. The strategy now consists in *taking the limit as* $q_0 \to \infty$ *right away, before iteration of formulas.* This is also the essential difference with respect to the method discussed in the previous section, where such a limit is taken at the very end of the proof, after infinitely many iterations. From (7.43) we get

$$\begin{aligned} \rho_n(q_1, \cdots, q_n) &= \rho e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \rho_{n-1}(q_2, \cdots, q_n) \\ &+ e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial \bar{q}_1} e^{W_{\bar{q}_1}(q_2, \cdots, q_n)} \\ &\cdot \rho_{n+1}(\bar{q}_1, q_2, \cdots, q_n, y_1) , \end{aligned} \tag{7.44}$$

where the double integral in the second term on the right hand side is *not* absolutely convergent, *but* it is well defined since it is equal to

$$\begin{aligned} & e^{-\beta W_{q_1}(q_2, \cdots, q_n)} \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \frac{\partial(-\beta\varphi(\bar{q}_1 - y_1))}{\partial \bar{q}_1} \\ & \cdot \left(e^{\beta W_{\bar{q}_1}(q_2, \cdots, q_n)} \rho_{n+1}(\bar{q}_1, q_2, \cdots, q_n, y_1) - \rho_2(\bar{q}_1, y_1)\rho_{n-1}(q_2, \cdots, q_n) \right) , \end{aligned} \tag{7.45}$$

the added term being null by the assumed rotation symmetry of the potential and of ρ_2. The exponential clustering (7.42) ensures that the double integral (7.45) is *absolutely convergent*, hence we can interchange the integrations to find

$$\begin{aligned}\rho_n(q_1,\cdots,q_n) &= (\rho-\gamma)e^{-\beta W_{q_1}(q_2,\cdots,q_n)}\rho_{n-1}(q_2,\cdots,q_n) \\ &+e^{-\beta W_{q_1}(q_2,\cdots,q_n)}\int_{\mathbb{R}^\nu}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\frac{\partial(-\beta\varphi(\bar{q}_1-y_1))}{\partial\bar{q}_1}e^{\beta W_{\bar{q}_1}(q_2,\cdots,q_n)} \\ &\cdot\rho_{n+1}(\bar{q}_1,q_2,\cdots,q_n,y_1)\ ,\end{aligned}\tag{7.46}$$

where we put

$$\begin{aligned}\gamma &= \int_{\mathbb{R}^\nu}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\rho_2(\bar{q}_1,y_1)\frac{\partial(-\beta\varphi(\bar{q}_1-y_1))}{\partial\bar{q}_1} \\ &\equiv \int_{B(q_1)}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\rho_2(\bar{q}_1,y_1)\frac{\partial(-\beta\varphi(\bar{q}_1-y_1))}{\partial\bar{q}_1}\ .\end{aligned}\tag{7.47}$$

Here $B(q)$ is the ball centered in q with radius equal to the range of φ, and the second equality is again true by the rotation symmetry. It is

$$\gamma\leq\tilde{A}\xi^2\ ,\tag{7.48}$$

where $\tilde{A}$ could be bounded in terms of β, the integral of $|\nabla\varphi|$ and the range of φ (or even in terms of β, the integral of φ and the number of changes of sign of $\frac{\partial\varphi}{\partial|q|}$).

The authors in [17] proceed by iteration of formula (7.46). Call for simplicity

$$\zeta=\rho-\gamma\ .\tag{7.49}$$

The first iteration gives

$$\begin{aligned}\rho_n(q_1,\cdots,q_n) &= \zeta e^{-\beta W_{q_1}(q_2,\cdots,q_n)}\Big[\rho_{n-1}(q_2,\cdots,q_n) \\ &-\int_{\mathbb{R}^\nu}dy_1(1-e^{-\beta\varphi(q_1-y_1)})\rho_n(q_2,\cdots,q_n,y_1)\Big] \\ &+e^{-\beta W_{q_1}(q_2,\ldots,q_n)}\int_{\mathbb{R}^\nu}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\int_{\mathbb{R}^\nu}dy_2\int_{-\infty}^{\bar{q}_1}d\bar{q}_2\prod_{j=1}^{2}\left(\frac{\partial}{\partial\bar{q}_j}(1-e^{-\beta\varphi(\bar{q}_j-y_j)})\right) \\ &\cdot e^{\beta W_{\bar{q}_2}(q_2,\ldots,q_n,y_1,y_2)}\rho_{n+2}(\bar{q}_2,q_2,\ldots,q_n,y_1,y_2)\ .\end{aligned}\tag{7.50}$$

If we iterate once again (7.46) in (7.50), the last term of (7.50) becomes

$$\begin{aligned}&\zeta e^{-\beta W_{q_1}(q_2,\ldots,q_n)}\int_{\mathbb{R}^\nu}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\int_{\mathbb{R}^\nu}dy_2\int_{-\infty}^{\bar{q}_1}d\bar{q}_2 \\ &\cdot\prod_{j=1}^{2}\left(\frac{\partial}{\partial\bar{q}_j}(1-e^{-\beta\varphi(\bar{q}_j-y_j)})\right)\rho_{n+1}(q_2,\ldots,q_n,y_1,y_2) \\ &-e^{-\beta W_{q_1}(q_2,\ldots,q_n)}\int_{\mathbb{R}^\nu}dy_1\int_{-\infty}^{q_1}d\bar{q}_1\int_{\mathbb{R}^\nu}dy_2\int_{-\infty}^{\bar{q}_1}d\bar{q}_2\int_{\mathbb{R}^\nu}dy_3\int_{-\infty}^{\bar{q}_2}d\bar{q}_3 \\ &\cdot\prod_{j=1}^{3}\left(\frac{\partial}{\partial\bar{q}_j}(1-e^{-\beta\varphi(\bar{q}_j-y_j)})\right)e^{\beta W_{\bar{q}_3}(q_2,\ldots,q_n,y_1,y_2,y_3)} \\ &\cdot\rho_{n+3}(\bar{q}_3,q_2,\ldots,q_n,y_1,y_2,y_3)\ .\end{aligned}\tag{7.51}$$

which is *not* equal to the formula in step 8) of [17] with $N = 2$; that is, the first term of (7.51) is not equal to

$$\zeta e^{-\beta W_{q_1}(q_2,\dots,q_n)} \frac{1}{2} \int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 (1 - e^{-\beta\varphi(q_1-y_1)})(1 - e^{-\beta\varphi(q_1-y_2)}) \cdot \rho_{n+1}(q_2, \dots, q_n, y_1, y_2) \,. \tag{7.52}$$

In fact, integrating in $\bar{q}_2$ the first term of (7.51) we have $\zeta e^{-\beta W_{q_1}(q_2,\dots,q_n)}$ times

$$\int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_2 \left(\frac{\partial}{\partial \bar{q}_1}(1 - e^{-\beta\varphi(\bar{q}_1-y_1)})\right)(1 - e^{-\beta\varphi(\bar{q}_1-y_2)}) \cdot \rho_{n+1}(q_2, \dots, q_n, y_1, y_2) \,; \tag{7.53}$$

in the last formula we can interchange the integrals in $\bar{q}_1$ and y_2 and this leads to

$$\int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{q_1} d\bar{q}_1 \left(\frac{\partial}{\partial \bar{q}_1}(1 - e^{-\beta\varphi(\bar{q}_1-y_1)})\right)(1 - e^{-\beta\varphi(\bar{q}_1-y_2)}) \cdot \rho_{n+1}(q_2, \dots, q_n, y_1, y_2) \tag{7.54}$$

but, since the integrals in y_1 and y_2 *are not* interchangeable, it is

$$\begin{aligned}
&\int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{q_1} d\bar{q}_1 (1 - e^{-\beta\varphi(\bar{q}_1-y_2)}) \frac{\partial(1 - e^{-\beta\varphi(\bar{q}_1-y_1)})}{\partial \bar{q}_1} \\
&\quad \cdot \rho_{n+1}(q_2, \dots, q_n, y_1, y_2) \\
&\neq \int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{q_1} d\bar{q}_1 (1 - e^{-\beta\varphi(\bar{q}_1-y_1)}) \frac{\partial(1 - e^{-\beta\varphi(\bar{q}_1-y_2)})}{\partial \bar{q}_1} \\
&\quad \cdot \rho_{n+1}(q_2, \dots, q_n, y_1, y_2)
\end{aligned} \tag{7.55}$$

in spite of the symmetry of ρ_{n+1}. This means that integration by parts of formula (7.54) does not lead to the desired term (7.52).

To convince the doubtful reader of (7.55), it will be sufficient to check it in the case $n = 1$, $q_1 = 0$, at first order in the Mayer expansion for ρ_2 (see (7.28), (7.29)):

$$\begin{aligned}
&\int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{0} d\bar{q} (1 - e^{-\beta\varphi(\bar{q}-y_2)}) \frac{\partial(1 - e^{-\beta\varphi(\bar{q}-y_1)})}{\partial \bar{q}} e^{-\beta\varphi(y_1-y_2)} \\
&\neq \int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{0} d\bar{q} (1 - e^{-\beta\varphi(\bar{q}-y_1)}) \frac{\partial(1 - e^{-\beta\varphi(\bar{q}-y_2)})}{\partial \bar{q}} e^{-\beta\varphi(y_1-y_2)} \,.
\end{aligned} \tag{7.56}$$

We shall do this here briefly and in a direct way for the one–dimensional case $\nu = 1$, and assuming for simplicity that $\varphi(q)$ is a monotonically decreasing function of $|q|$, so that the three factors in the integrand are monotonic functions of the absolute value of their arguments. We refer to Appendix F for a proof of (7.56) valid in any dimension. First of all, notice that by symmetry we can restrict the integrals in y_1 (in any dimension) in both sides of (7.56) to the ball $B(0)$; in fact, fixed y_1

outside $B(0)$, for any value of the couple $(\bar{q}, y_2)$ we can find another one that gives opposite contribution to the integrals. To do that, reflect the couple $(\bar{q}, y_2)$ by the ($(\nu-1)-$dimensional) axis passing through y_1 and perpendicular to the line $\overrightarrow{-\infty 0}$. Secondly observe that, in the monotonicity assumption, the left hand side in (7.56) is strictly positive, since the only negative contributions are exactly cancelled by the same symmetry argument. Finally, we shall show that in the case $\nu = 1$ the right hand side in (7.56) is strictly negative: write

$$\begin{aligned}
&\int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{0} d\bar{q}(1-e^{-\beta\varphi(\bar{q}-y_1)})\frac{\partial(1-e^{-\beta\varphi(\bar{q}-y_2)})}{\partial\bar{q}} e^{-\beta\varphi(\bar{q}-y_2)} \qquad (7.57)\\
&= \int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{0} d\bar{q}(1-e^{-\beta\varphi(\bar{q}-y_1)})\frac{\partial(1-e^{-\beta\varphi(\bar{q}-y_2)})}{\partial\bar{q}}\\
&\quad - \int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^{0} d\bar{q}(1-e^{-\beta\varphi(\bar{q}-y_1)})\frac{\partial(1-e^{-\beta\varphi(\bar{q}-y_2)})}{\partial\bar{q}}(1-e^{-\beta\varphi(y_1-y_2)})\ .
\end{aligned}$$

The integral in y_2 in the second line is equal to zero. The integrand in the third line changes sign when we exchange $\bar{q}$ and y_2, hence what remains in one dimension is

$$\begin{aligned}
&-\int_{-d}^{+d} dy_1 \int_{0}^{\infty} dy_2 \int_{-\infty}^{0} d\bar{q}(1-e^{-\beta\varphi(\bar{q}-y_1)})\frac{\partial(1-e^{-\beta\varphi(\bar{q}-y_2)})}{\partial\bar{q}}(1-e^{-\beta\varphi(y_1-y_2)})\\
&< 0\ . \qquad (7.58)
\end{aligned}$$

The additional terms missing in the formula in step 8) of [17], obtained by repeated iteration of (7.46), give higher order corrections to the constant ζ, and all these (infinitely many) corrections lead to a definition of the activity. However, to construct the correct expansion for the activity, it is convenient to keep the inverse order of integration in formula (7.46): that is to iterate Eq. (7.44), as we show in what follows. Let us use the short notations

$$\begin{aligned}
&\mathcal{K}_h^{(1)} = \frac{(-1)^h}{h!}\int_{\mathbb{R}^{\nu h}} dy_1\cdots dy_h \prod_{j=1}^{h}\Big(1-e^{-\beta\varphi(y_j)}\Big)\rho_h(y_1,\cdots,y_h)\ , \qquad \mathcal{K}_0^{(1)} = 1\ ,\\
&\mathcal{K}_h^{(n)}(q_1,\cdots,q_n) = \frac{(-1)^h}{h!}\int_{\mathbb{R}^{\nu h}} dy_1\cdots dy_h \prod_{j=1}^{h}\Big(1-e^{-\beta\varphi(q_1-y_j)}\Big)\\
&\qquad \cdot\rho_{n-1+h}(q_2,\cdots,q_n,y_1,\cdots,y_h)\ , \qquad\qquad n\geq 2\ , \qquad (7.59)
\end{aligned}$$

and the convention $0! = 1$. The result is the following

Lemma 7.3.1 *After N iterations of formula (7.44) we have*

$$\begin{aligned}
\rho_n(q_1,\cdots,q_n) &= e^{-\beta W_{q_1}(q_2,\cdots,q_n)}\sum_{h=0}^{N}\zeta^{(N-h)}\mathcal{K}_h^{(n)}(q_1,\cdots,q_n) \qquad (7.60)\\
&\quad + R_{n,N}(q_1,\cdots,q_n)\ ,
\end{aligned}$$

where the remainder $R_{n,N}$ is given by

$$\begin{aligned}
R_{n,N}(q_1,\ldots,q_n) := {} & (-1)^{N+1} e^{-\beta W_{q_1}(q_2,\ldots,q_n)} \\
& \cdot \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^{\bar{q}_1} d\bar{q}_2 \int_{\mathbb{R}^\nu} dy_2 \ldots \int_{-\infty}^{\bar{q}_N} d\bar{q}_{N+1} \int_{\mathbb{R}^\nu} dy_{N+1} \\
& \cdot e^{\beta W_{\bar{q}_{N+1}}(q_2,\ldots,q_n,y_1,\ldots,y_{N+1})} \prod_{j=1}^{N+1} \left(\frac{\partial}{\partial \bar{q}_j} (1 - e^{-\beta\varphi(\bar{q}_j - y_j)}) \right) \\
& \cdot \rho_{n+N+1}(\bar{q}_{N+1}, q_2, \ldots, q_n, y_1, \ldots, y_{N+1}) \ ,
\end{aligned} \tag{7.61}$$

and the coefficients $\zeta^{(N-h)}$ are defined by

$$\begin{aligned}
\zeta^{(N-h)} &= \rho \sum_{n=0}^{N-h} C^{(n)} \ , \\
C^{(n)} &= \sum_{\substack{j_1, j_2 \cdots \geq 0 \\ \sum_{i\geq 1} i j_i = n}} (-1)^{\sum_{i\geq 1} j_i} \frac{(\sum_{i\geq 1} j_i)!}{\prod_{i\geq 1} j_i!} \prod_{i\geq 1} (\mathcal{K}_i^{(1)})^{j_i} \ .
\end{aligned} \tag{7.62}$$

Notice that $C^{(n)}$ can be obtained by expanding formula (7.27) and collecting all the terms of order n.

Proof of Lemma 7.3.1. For $N = 0$ Eq. (7.61) coincides with (7.44). The inductive step follows from direct substitution provided the following formula holds:

$$\begin{aligned}
& (-1)^N \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^{\bar{q}_1} d\bar{q}_2 \int_{\mathbb{R}^\nu} dy_2 \ldots \int_{-\infty}^{\bar{q}_{N-1}} d\bar{q}_N \int_{\mathbb{R}^\nu} dy_N \\
& \qquad \cdot \prod_{j=1}^{N} \left(\frac{\partial}{\partial \bar{q}_j} (1 - e^{-\beta\varphi(\bar{q}_j - y_j)}) \right) \rho_{n+N-1}(q_2, \ldots, q_n, y_1, \ldots, y_N) \\
& = \sum_{h=0}^{N} C^{(N-h)} \mathcal{K}_h^{(n)}(q_1, \cdots, q_n) \ .
\end{aligned} \tag{7.63}$$

This equality follows from explicit computation of the line integrals in the left hand side, which can be performed again recursively starting from the innermost. At each step, before the explicit integration, we need to exchange the integration order $\int d\bar{q} \int dy \to \int dy \int d\bar{q}$: this produces higher order terms contributing to formula (7.62).

Notice that for $N = 0$ Eq. (7.63) reduces to the identity

$$\rho_{n-1}(q_2, \cdots, q_n) = \mathcal{K}_0^{(n)}(q_1, \cdots, q_n).$$

Assume that (7.63) is true with N replaced by $N-1$. Then

$$
\begin{aligned}
&(-1)^N \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^{\bar{q}_1} d\bar{q}_2 \int_{\mathbb{R}^\nu} dy_2 \dots \int_{-\infty}^{\bar{q}_{N-1}} d\bar{q}_N \int_{\mathbb{R}^\nu} dy_N \\
&\quad \cdot \prod_{j=1}^{N} \left(\frac{\partial}{\partial \bar{q}_j} (1 - e^{-\beta\varphi(\bar{q}_j - y_j)}) \right) \rho_{n+N-1}(q_2, \dots, q_n, y_1, \dots, y_N) \\
&= - \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \left(\frac{\partial}{\partial \bar{q}_1} (1 - e^{-\beta\varphi(\bar{q}_1 - y_1)}) \right) \\
&\quad \cdot \sum_{h=0}^{N-1} C^{(N-1-h)} \mathcal{K}_h^{(n+1)}(\bar{q}_1, q_2, \cdots, q_n, y_1) \\
&= \sum_{h=0}^{N-1} C^{(N-1-h)} \frac{(-1)^{h+1}}{h!} \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^{\nu(h+1)}} dy_1 \cdots dy_{h+1} \\
&\quad \cdot \left(\frac{\partial}{\partial \bar{q}_1} (1 - e^{-\beta\varphi(\bar{q}_1 - y_1)}) \right) \prod_{j=2}^{h+1} (1 - e^{-\beta\varphi(\bar{q}_1 - y_j)}) \\
&\quad \cdot [\rho_{n+h}(q_2, \cdots, q_n, y_1, \cdots, y_{h+1}) - \rho_{n-1}(q_2, \cdots, q_n) \rho_{h+1}(y_1, \cdots, y_{h+1})] \ ,
\end{aligned}
\tag{7.64}
$$

where the subtracted terms in the last formula are null by the symmetry assumption *b)*: fixed $\bar{q}_1$, for any value of the vector $(y_1, \cdots, y_{h+1})$ we can find another one that gives opposite contribution to the integral, by reflecting $(y_1, \cdots, y_{h+1})$ through the $((\nu-1)-$dimensional) axis passing through $\bar{q}_1$ and perpendicular to the line $\overrightarrow{-\infty 0}$. Assumption *c)* and the finiteness of the range imply that the resulting multiple integrals are absolutely convergent, so that taking inside the integration $\int_{-\infty}^{q_1} d\bar{q}_1$ and computing it by parts we get

$$
\begin{aligned}
&(-1)^N \int_{-\infty}^{q_1} d\bar{q}_1 \int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^{\bar{q}_1} d\bar{q}_2 \int_{\mathbb{R}^\nu} dy_2 \dots \int_{-\infty}^{\bar{q}_{N-1}} d\bar{q}_N \int_{\mathbb{R}^\nu} dy_N \\
&\quad \cdot \prod_{j=1}^{N} \left(\frac{\partial}{\partial \bar{q}_j} (1 - e^{-\beta\varphi(\bar{q}_j - y_j)}) \right) \rho_{n+N-1}(q_2, \dots, q_n, y_1, \dots, y_N) \\
&= \sum_{h=0}^{N-1} C^{(N-1-h)} \frac{(-1)^{h+1}}{(h+1)!} \int_{\mathbb{R}^{\nu(h+1)}} dy_1 \cdots dy_{h+1} \prod_{j=1}^{h+1} (1 - e^{-\beta\varphi(q_1 - y_j)}) \\
&\quad \cdot [\rho_{n+h}(q_2, \cdots, q_n, y_1, \cdots, y_{h+1}) - \rho_{n-1}(q_2, \cdots, q_n) \rho_{h+1}(y_1, \cdots, y_{h+1})] \\
&= \sum_{h=1}^{N} C^{(N-h)} \mathcal{K}_h^{(n)}(q_1, \cdots, q_n) - \sum_{p=1}^{N} \mathcal{K}_p^{(1)} C^{(N-p)} \mathcal{K}_0^{(n)}(q_1, \cdots, q_n) \ .
\end{aligned}
\tag{7.65}
$$

We have

$$
\begin{aligned}
&-\sum_{p=1}^{N}\mathcal{K}_p^{(1)}C^{(N-p)} \\
&\equiv -\sum_{p=1}^{N}\mathcal{K}_p^{(1)}\sum_{\substack{j_1,j_2\cdots\geq 0\\ \sum_{i\geq 1} i j_i = N-p}}(-1)^{\sum_{i\geq 1} j_i}\frac{(\sum_{i\geq 1} j_i)!}{\prod_{i\geq 1} j_i!}\prod_{i\geq 1}(\mathcal{K}_i^{(1)})^{j_i} \\
&=\sum_{p=1}^{N}\sum_{\substack{j_1,j_2\cdots\geq 0 | j_p\geq 1,\\ \sum_{i\geq 1} i j_i = N}}(-1)^{\sum_{i\geq 1} j_i}\frac{\Big((\sum_{i\geq 1} j_i)-1\Big)!}{(\prod_{1\leq i\neq p} j_i!)(j_p-1)!}\prod_{i\geq 1}(\mathcal{K}_i^{(1)})^{j_i} \\
&=\sum_{\substack{j_1,j_2\cdots\geq 0\\ \sum_{i\geq 1} i j_i = N}}(-1)^{\sum_{i\geq 1} j_i}\prod_{i\geq 1}(\mathcal{K}_i^{(1)})^{j_i}\sum_{\substack{p=1 \text{ s.t.}\\ j_p\geq 1}}^{N}\frac{\Big((\sum_{i\geq 1} j_i)-1\Big)!}{(\prod_{1\leq i\neq p} j_i!)(j_p-1)!} \\
&=\sum_{\substack{j_1,j_2\cdots\geq 0\\ \sum_{i\geq 1} i j_i = N}}(-1)^{\sum_{i\geq 1} j_i}\frac{(\sum_{i\geq 1} j_i)!}{\prod_{i\geq 1} j_i!}\prod_{i\geq 1}(\mathcal{K}_i^{(1)})^{j_i} \\
&\equiv C^{(N)}\ ,
\end{aligned}
\tag{7.66}
$$

which, substituted in (7.65), concludes the proof. □

The convergence of the iteration procedure that has been set by the previous lemma is handled in assumptions *a)* and *b)*. In fact, the remainder $R_{n,N}(q_1,\ldots,q_n)$ can be bounded as outlined in [17], using the cluster property, by

$$
|R_{n,N}(q_1,\ldots,q_n)|\leq (A\xi)^{n+N+1}\ , \tag{7.67}
$$

where A is a suitable constant depending on β, C, κ and φ. So it goes to zero when $N\to\infty$ if ξ is small enough. For what concerns the constant $\zeta^{(N-h)}$, notice that

$$
\mathcal{K}_h^{(1)}\leq\frac{(I_\beta\xi)^h}{h!}, \tag{7.68}
$$

where I_β is defined as in (7.30); hence

$$
\begin{aligned}
C^{(n)} &\leq \sum_{\substack{j_1,j_2\cdots\geq 0\\ \sum_{i\geq 1} i j_i = n}}\frac{(\sum_{i\geq 1} j_i)!}{\prod_{i\geq 1} j_i!}\prod_{i\geq 1}\left(\frac{(I_\beta\xi)^i}{i!}\right)^{j_i} \\
&\leq (I_\beta\xi)^n\sum_{\substack{j_1,j_2\cdots\geq 0\\ \sum_{i\geq 1} i j_i = n}}\frac{(\sum_{i\geq 1} j_i)!}{\prod_{i\geq 1}(i!)^{j_i} j_i!}\leq(\overline{C}\xi)^n\ ,
\end{aligned}
\tag{7.69}
$$

the last sum being exponentially bounded in n. Therefore for ξ small we can take the limit $N\to\infty$ in (7.62), and we obtain that Equation (7.61) converges to the

Kirkwood–Salsburg equations (7.15) with activity $z = O(\xi)$ defined by the absolutely convergent expansion

$$z = \rho \sum_{n=0}^{\infty} C^{(n)} \ , \tag{7.70}$$

which is in turn equivalent to the first of the Kirkwood–Salsburg equations, Eq. (7.27).

Remark. We have the following differences with respect to the method presented in Section 7.2: *(i)* the rate of convergence of the iteration is exponential, Eq. (7.67) (instead of factorial, see (Eq. (7.24)): this implies convergence for sufficiently small values of ξ, see also the comment after the proof of Theorem 7.2.1; *(ii)* rotation invariance and strong cluster assumptions are strictly needed to control the convergence of the integrals over the unbounded domains of integration: this makes the method not suitable to extend the result to different kinds of boundary condition, such as the one discussed in Section 7.2.1; *(iii)* the radius of convergence of the procedure is at least $1/A$, where A is not uniformly bounded in the maximum of the potential (see the proof of Proposition 8.0.1 in the following chapter).

Chapter 8

The hard core limit

In this section we deal with the infinite system of hard core particles with diameter $d > 0$, stating some consequences of the discussion of Section 7.2. For this we mean the case of an Hamiltonian $H(X)$ defined by (7.1) with

$$\varphi_d(q) = \begin{cases} \infty, & |q| < d \\ 0, & |q| \geq d \end{cases} ,$$

over the phase space $\mathcal{H}_d = \{X = \{x_i\}_{i=0}^{\infty} = \{(q_i, p_i)\}_{i=0}^{\infty}, x_i \in \mathbb{R}^\nu \times \mathbb{R}^\nu \mid |q_i - q_j| \geq d \text{ for } i \neq j\}$. Definitions of Section 7.1 can be easily extended: [2]. In particular, a state is a probability measure on the Borel sets of $\mathcal{H}_d$ having correlation functions

$$\overline{\rho}_n : \mathcal{H}_d^{(n)} \to \mathbb{R}^+ , \tag{8.1}$$

where

$$\mathcal{H}_d^{(n)} = \Big\{ \{x_i\}_{i=0}^{n} = \{(q_i, p_i)\}_{i=0}^{n}, x_i \in \mathbb{R}^\nu \times \mathbb{R}^\nu \mid |q_i - q_j| > d \text{ for } i \neq j \Big\} . \tag{8.2}$$

The state μ is smooth if it is in $C(\overline{\mathcal{H}}_d^{(n)})$ and piecewise $C^1(\mathcal{H}_d^{(n)})$, and satisfies (7.4) and similar bound for the derivative.

Let

$$\Omega_i(q_1, \cdots, q_n) = \{\omega \in S^{\nu-1} \mid |q_i + dw - q_j| > d \text{ for every } j \in (1, \cdots, n), j \neq i\} . \tag{8.3}$$

Following [6][1], we also say that μ is a stationary solution of the hard core BBGKY

[1]Cercignani derives the non stationary hierarchy for a finite system of hard spheres in a box, assuming smothness of the correlations at all times. There exists also a rigorous derivation that can be found in [23]. The problems concerning the infinite system dynamics are treated in [4].

hierarchy if, for $n \geq 1$,

$$\sum_{i=1}^{n} p_i \cdot \nabla_{q_i} \overline{\rho}_n(x_1, \cdots, x_n) \tag{8.4}$$
$$= -d^{\nu-1} \sum_{i=1}^{n} \int_{\Omega_i(q_1,\cdots,q_n)\times\mathbb{R}^\nu} d\omega d\pi \ \omega \cdot (p_i - \pi) \overline{\rho}_{n+1}(x_1, \cdots, x_n, q_i + d\omega, \pi)$$

for any $(x_1, \cdots, x_n) \in \mathcal{H}_d^{(n)}$, where ω varies over $\Omega_i(q_1, \cdots, q_n)$, π varies in $\mathbb{R}^\nu$, and $d\omega$ denotes the surface element on the unit sphere (for $\nu = 1$ it reduces to $\sum_{\omega=\pm1}$). The equations should be complemented with the boundary conditions imposing that the correlation functions take the same value on configurations that correspond to the incoming and outcoming state of a collision.

In the case of a Mawxellian state we have spatial correlation functions

$$\rho_n : \mathbb{R}_d^{\nu n} \to \mathbb{R}^+ \ , \tag{8.5}$$

where

$$\mathbb{R}_d^{n\nu} = \{(q_1, \cdots, q_n) \in \mathbb{R}^{\nu n} \mid |q_i - q_j| > d \text{ for } i \neq j\} \ , \tag{8.6}$$

with $\rho_n \in C(\overline{\mathbb{R}}_d^{\nu n})$, piecewise $C^1(\mathbb{R}_d^{\nu n})$ and satisfying the hierarchy

$$\nabla_{q_1} \rho_n(q_1, \cdots, q_n) = -d^{\nu-1} \int_{\Omega_1(q_1,\cdots,q_n)} d\omega \omega \rho_{n+1}(q_1, \cdots, q_n, q_1 + d\omega) \ , \tag{8.7}$$

which is the analogous of (7.11) for the hard core potential. Observe that in this case, if the state is also invariant, the equations are parametrized by only one positive constant, $\rho \equiv \rho_1(q_1)$ (β does not appear). Finally, notice that the cluster property is formulated as in (7.14) for the functions defined on $\mathbb{R}_d^{\nu(n+m)}$.

The direct integration procedures established in the previous chapter cannot be applied to solve the hierarchy (8.7), the difficulty coming from the presence of "holes" in the phase space (notice that, in the proof of Theorem 7.2.1 in Section 7.2, as well as in the proof Lemma 7.3.1 in Section 7.3, the integration paths necessarily cross regions contained in the range of interaction of the other particles involved in the formula). However, the solution of (8.7) describing the equilibrium correlation functions of the hard core system, defined (uniquely for ρ small) via its corresponding Kirkwood–Salsburg equations, can be approximated with solutions of the smooth hierarchies (7.11), with few restrictions on the form of the regular potentials that can be used.

More precisely, let $\varphi^{(\varepsilon)} \in C^1(\mathbb{R}^\nu), \varepsilon > 0$, be a family of smooth positive potentials with compact support, depending only on $|q|, q \in \mathbb{R}^\nu$, and converging pointwise to the hard core potential:

$$\varphi^{(\varepsilon)}(q) \underset{\varepsilon\to0}{\longrightarrow} \varphi_d(q), \qquad \text{for } |q| \neq d \ . \tag{8.8}$$

For brevity, we will denote $\mathbf{M}^{(\beta,\xi)}$ the set of smooth invariant states on $\mathcal{H}$ which are Maxwellian with parameter β, and obey the estimates (7.12)–(7.14) (with possibly different constants C_n, C). We call $B_d(q)$ the ball with radius d and center $q \in \mathbb{R}^\nu$, and

$$\mathbb{R}_d^{m\nu}(q_1, \cdots, q_n) = \left\{ (y_1, \cdots, y_m) \in \mathbb{R}_d^{\nu m} \;\middle|\; (q_1, \cdots, q_n, y_1, \cdots, y_m) \in \mathbb{R}_d^{\nu(n+m)} \right\} . \tag{8.9}$$

Then the following holds:

Proposition 8.0.1 *Fix $\beta > 0$, and sufficiently small $\rho > 0$. Then there exists a (small) constant $\xi > \rho$ such that:*

(i) for any $\varepsilon > 0$ there is a unique state in $\mathbf{M}^{(\beta,\xi)}$ with spatial correlation functions $\{\rho_n^{(\varepsilon)}\}_{n=1}^\infty$ solving the hierarchy (7.11) with potential $\varphi^{(\varepsilon)}$, and $\rho_1^{(\varepsilon)}(q_1) \equiv \rho$;

(ii) it is $|\rho_n^{(\varepsilon)}(q_1, \cdots, q_n)| \leq (2\xi)^n e^{-\beta \sum_{i \neq j} \varphi^{(\varepsilon)}(q_i - q_j)}$ for all $\varepsilon > 0, n \geq 1$ and $(q_1, \cdots, q_n) \in \mathbb{R}^{\nu n}$; moreover,

$$\rho_n^{(\varepsilon)}(q_1, \cdots, q_n) \underset{\varepsilon \to 0}{\longrightarrow} \rho_n(q_1, \cdots, q_n) \tag{8.10}$$

uniformly in every compact subset of $\mathbb{R}_d^{\nu n}$, where the functions $\rho_n : \mathbb{R}_d^{\nu n} \to \mathbb{R}^+$ are given by the hard core Kirkwood–Salsburg equations:

$$\begin{aligned} \rho_n(q_1, \cdots, q_n) = z\Big[&\rho_{n-1}(q_2, \cdots, q_n) \\ &+ \sum_{m=1}^\infty \frac{(-1)^m}{m!} \int_{\mathbb{R}_d^{m\nu}(q_2, \cdots, q_n) \bigcap (B_d(q_1))^m} dy_1 \cdots dy_m \\ &\cdot \rho_{n-1+m}(q_2, \cdots, q_n, y_1, \cdots, y_m)\Big] . \end{aligned} \tag{8.11}$$

(iii) the limit functions ρ_n satisfy the hard core hierarchy (8.7).

Notice that the sum in the right hand side of (8.11) is finite, because of the hard core exclusion. From points *(ii)* and *(iii)* of the proposition, and the known theory of equations (8.11) for small densities, it follows that the limit functions ρ_n provide a smooth, invariant, Maxwellian state on $\mathcal{H}_d$ with correlation functions $\overline{\rho}_n$ on $\mathcal{H}_d^{(n)}$ of the form (7.8), obeying the stationary hard core BBGKY hierarchy (8.4), and cluster boundary conditions.

It would be interesting to find an iterative procedure that integrates Eq. (8.7) directly, as we are able to do in the smooth case. This is, as far as we know, an open problem. A direct integration can be carried out for ρ small in the case $\nu = 1$: we discuss it in Section 8.1.

Proof of Proposition 8.0.1. Applying the direct statement of the Theorem in Section 7.2, we have that any state in $\mathbf{M}^{(\beta,\xi)}$ with fixed density $\rho < \xi$, solving the stationary BBGKY hierarchy with interaction $\varphi^{(\varepsilon)}$ (or, equivalently, Eq. (7.11) with interaction $\varphi^{(\varepsilon)}$), satisfies also Eq. (7.15) with the same interaction, for some value of the activity z_ε. By the proof of the Corollary in Section 7.2, this last set of equations has a unique solution if ξ is taken as in (7.33) (notice that this does not follow from the method of [17], since the estimate of the remainder term in step 9), page 283 of [17] is not uniform in the maximum of the potential, hence in ε). Thus point *(i)* is proved by chosing ξ (hence ρ) in such a way that

$$\xi < \frac{1}{2e \sup_{\varepsilon>0} \int_{\mathbb{R}^\nu} \left(1 - e^{-\beta\varphi^{(\varepsilon)}(x)}\right) dx} \ . \tag{8.12}$$

The solution $\rho_n^{(\varepsilon)}$ for given ε can be expanded in (absolutely convergent) power series of the activity, so that we have formula (7.28) with z replaced by z_ε, a superscript (ε) added to ρ_n and coefficients of the expansions $c_{1,p}^{(\varepsilon)}, c_{n,p}^{(\varepsilon)}$ defined by Eq. (7.29) with potential $\varphi^{(\varepsilon)}$. Since $\varphi^{(\varepsilon)}$ is positive, it turns out (see [21]) that the coefficients of the series expansions have alternating signs, and that the same expansions have the *alternating bound property* [35], which means in particular that, for $z_\varepsilon > 0$ (which is certainly true if ρ is small enough for all $\varepsilon > 0$), they can be bounded with their leading terms as:

$$\rho_n^{(\varepsilon)} < z_\varepsilon^n c_{n,n-1} = z_\varepsilon^n e^{-\beta \sum_{i<j}^{0,n} \varphi^{(\varepsilon)}(q_i - q_j)} \ . \tag{8.13}$$

This, together with (8.12) and (7.27), gives the required estimate.

Using now this bound and assuming by induction on p that $c_{n,p}^{(\varepsilon)} \to c_{n,p}^{(0)}$ as $\varepsilon \to 0$, where $c_{n,p}^{(0)}$ are the coefficients of the formal expansion obtained by iteration of Eq. (8.11), we obtain from (7.29) that for $|q_i - q_j| > d$:

$$\begin{aligned}
&\lim_{\varepsilon\to 0} c_{n,p+1}^{(\varepsilon)}(q_1, \cdots, q_n) = \Big[\delta_{n>1} c_{n-1,p}(q_2, \cdots, q_n) \\
&+ \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \int_{\mathbb{R}_d^{m\nu}(q_2,\cdots,q_n) \bigcap (B_d(q_1))^m} dy_1 \cdots dy_k \\
&\qquad \cdot c_{n+k-1,p}^{(0)}(q_2, \cdots, q_n, y_1, \cdots, y_k)\Big] \\
&\equiv c_{n,p+1}^{(0)}(q_1, \cdots, q_n) \ .
\end{aligned} \tag{8.14}$$

This concludes the proof of point *(ii)*.

Point *(iii)* is now a particular case of the following Lemma, which is the analogous of the converse statement of the Theorem in Section 7.2:

Lemma 8.0.2 *If a smooth Maxwellian state on $\mathcal{H}_d$ satisfies (8.11), then it is a stationary solution of the hard core BBGKY, Eq. (8.4).*

Proof of the Lemma. We compute the gradient with respect to q_1 of expression (8.11), in a configuration $(q_1, \cdots, q_n) \in \mathbb{R}_d^{\nu n}$. Remind that the series in the right hand side is actually a finite sum. We have

$$\begin{aligned} &\nabla_{q_1} \rho_n(q_1, \cdots, q_n) \qquad (8.15)\\ &= z \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} \nabla_{q_1} \int_{\mathbb{R}_d^{k\nu}(q_2,\cdots,q_n) \bigcap (B_d(q_1))^k} dy_1 \cdots dy_k \rho_{n-1+k}(q_2, \cdots, q_n, y_1, \cdots, y_k) \\ &= z \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} k \int_{\mathbb{R}_d^{(k-1)\nu}(q_2,\cdots,q_n) \bigcap (B_d(q_1))^{k-1}} dy_1 \cdots dy_k \\ &\quad \cdot \nabla_{q_1} \int_{\mathbb{R}_d^{\nu}(q_2,\cdots,q_n,y_1,\cdots,y_{k-1}) \bigcap B_d(q_1)} dy^* \rho_{n-1+k}(q_2, \cdots, q_n, y^*, y_1, \cdots, y_{k-1}) \,, \end{aligned}$$

where the second equivalence holds by symmetry in the exchange of particle labels and by uniform convergence of the integrals. The integral in the last line of the formula is extended on a region which has positive volume for sufficiently small k, and piecewise smooth boundary: the ball centered in q_1 minus the union of the balls centered in the points $q_2, \cdots, q_n, y_1, \cdots, y_{k-1}$. Being the integrand function $\rho_{n-1+k}(\cdots, y^*, \cdots,)$ continuous in the closure of its domain, it is easy to see that the gradient with respect to q_1 of such an integral is given by the surface integral of the restriction of the function over the part of the boundary of $B_d(q_1)$ that remains ouside the other balls, i.e. using the notations of (2.11) and (8.4):

$$d^{\nu-1} \int_{\Omega_1(q_1,\cdots,q_n,y_1,\cdots,y_{k-1})} d\omega \omega \rho_{n-1+k}(q_2, \cdots, q_n, q_1 + d\omega, y_1, \cdots, y_{k-1}) \,.$$

Interchanging the integrations we find

$$\begin{aligned} &\nabla_{q_1} \rho_n(q_1, \cdots, q_n) \qquad (8.16)\\ &= d^{\nu-1} \int_{\Omega_1(q_1,\cdots,q_n)} d\omega \omega z \sum_{k=1}^{\infty} \frac{(-1)^k}{k!} k \\ &\cdot \int_{\mathbb{R}_d^{(k-1)\nu}(q_2,\cdots,q_n,q_1+d\omega) \bigcap (B_d(q_1))^{k-1}} dy_1 \cdots dy_{k-1} \\ &\quad \cdot \rho_{n-1+k}(q_2, \cdots, q_n, q_1 + d\omega, y_1, \cdots, y_{k-1}) \,. \end{aligned}$$

Using that (8.11) holds also, by continuity, over the boundary of $\mathbb{R}_d^{\nu n}$, we recognize function

$$-\rho_{n+1}(q_1, q_2, \cdots, q_n, q_1 + d\omega) \qquad (8.17)$$

in the above expression, thus obtaining Eq. (8.7). Taking into account the assumption (7.8), Eq. (8.4) follows. □

8.1 Integration of the hard rod hierarchy

In this section we shall find the unique and *explicit* solution to the one–dimensional hard rod hierarchy

$$
\begin{aligned}
&\frac{\partial \rho_n}{\partial q_1}(q_1,\cdots,q_n) = \chi_{q_1}(|q_1-a-q_i|\geq d)\rho_{n+1}(q_1,\cdots,q_n,q_1-d)\\
&\qquad -\chi_{q_1}(|q_1+a-q_i|\geq d)\rho_{n+1}(q_1,q_2,\cdots,q_n,q_1+d)\ ,\\
&(q_1,\cdots,q_n)\in\mathbb{R}^n_d\ ,\\
&\chi_x(\mathcal{A}) = 1 \text{ if } x\in\mathcal{A} \text{ and } 0 \text{ otherwise,}
\end{aligned}
\tag{8.18}
$$

with the assumptions of invariance under translation and permutation of particles, sufficiently small $\rho \equiv \rho_1$ (precisely $\rho < 1/d$), cluster property (7.14), continuity over $\overline{\mathbb{R}}^n_d$ and piecewise C^1 regularity on $\mathbb{R}^n_d$. The special feature of this case is the existence of an explicit form for the equilibrium correlation functions, [29]. In what follows, we derive this expressions from the hierarchy by direct integration and without going through the corresponding Kirkwood–Salsburg equations.

To do this, we can follow the procedure of [17] in a rather natural way by ordering the particles from left to right: $q_i \leq q_{i+1}-d$; hence we start rewriting

$$
\begin{aligned}
&\frac{\partial \rho_n}{\partial q_1}(q_1,\cdots,q_n) = \rho_{n+1}(q_1-d,q_1,\cdots,q_n)\\
&\qquad -\chi(q_1\leq q_2-2d)\rho_{n+1}(q_1,q_1+d,q_2,\cdots,q_n)\ ,\\
&q_i\in\mathbb{R}\ ,\qquad q_1<q_{i+1}-d\ .
\end{aligned}
\tag{8.19}
$$

Now we choose $q_0 << q_1$ and we integrate from q_0 to q_1:

$$
\begin{aligned}
&\rho_n(q_1,q_2,\cdots,q_n) = \rho_n(q_0,q_2,\cdots,q_n) \qquad (8.20)\\
&+\int_{q_0}^{q_1} d\bar{q}\Big(\rho_{n+1}(\bar{q}-d,\bar{q},q_2\cdots,q_n) - \chi(\bar{q}\leq q_2-2d)\rho_{n+1}(\bar{q},\bar{q}+d,q_2,\cdots,q_n)\Big)\\
&\quad = \rho_n(q_0,q_2,\cdots,q_n) + \int_{q_0}^{q_0+d} d\bar{q}\rho_{n+1}(\bar{q}-d,\bar{q},q_2\cdots,q_n)\\
&-\int_{q_1}^{q_1+d} d\bar{q}\chi(\bar{q}\leq q_2-d)\rho_{n+1}(\bar{q},\bar{q}-d,q_2,\cdots,q_n)\ ,
\end{aligned}
$$

where we used again symmetry the symmetry in the particle labels to split the integral in the second equality. Sending q_0 to $-\infty$ gives

$$
\begin{aligned}
&\rho_n(q_1,q_2,\cdots,q_n) = \Big(\rho + d\rho_2(d)\Big)\rho_{n-1}(q_2,\cdots,q_n)\\
&\qquad -\int_{q_1}^{q_1+d} d\bar{q}\chi(\bar{q}\leq q_2-d)\rho_{n+1}(\bar{q},\bar{q}-d,q_2,\cdots,q_n)\ ,\\
&\rho_2(d) := \rho_2(q,q+d)\ ,
\end{aligned}
\tag{8.21}
$$

having used the cluster property and the translation invariance.

Call $R := \rho + d\rho_2(d)$. Iterating once the above equation we have

$$\begin{aligned}
&\rho_n(q_1, q_2, \cdots, q_n) \\
&\quad = R\Big[\rho_{n-1}(q_2, \cdots, q_n) - \int_{q_1}^{q_1+d} d\bar{q}\chi(\bar{q} \le q_2 - d)\rho_n(\bar{q}, q_2, \cdots, q_n)\Big] \ .
\end{aligned} \tag{8.22}$$

We stress again that the above explained procedure does not lead to the Kirkwood–Salsburg equations, since the extracted constant R is different from the activity of the hard rod gas (which is known to be given by $z = Re^{Rd}$, see for instance [29]). Nevertheless the set of equations (8.22) can be solved explicitly for every n, starting from $n = 2$ (the equation for $n = 1$ is useless in this case), as we will show below. In fact, the simple structure of Eq. (8.22) allows to construct easily ρ_n from ρ_{n-1} : this structure is due to the strong symmetry used to split the integral in the second equality of (8.20), and it seems to have no analogue in higher dimensions.

We start with the $n = 2$ case.

Proposition 8.1.1 *Call $x = |q_2 - q_1|$, $x \ge d$. The solution of (8.18) for $n = 2$ is*

$$\rho_2(x) = \rho \sum_{k=1}^{[x/d]} \Big(\frac{\rho}{1-\rho d}\Big)^k \frac{(x-kd)^{k-1}}{(k-1)!} e^{-\frac{(x-kd)\rho}{1-\rho d}} \ . \tag{8.23}$$

Proof. Formula (8.22) for $n = 2$ and $q_1 = q_2 - d$ gives

$$\rho_2(d) = \frac{\rho^2}{1-\rho d}, \qquad R = \frac{\rho}{1-\rho d} \ . \tag{8.24}$$

Moreover, it implies

$$\begin{aligned}
&\frac{d\rho_2}{dx}(x) = -R\rho_2(x) \ , \qquad d < x < 2d \\
&\frac{d\rho_2}{dx}(x) = R\Big(- \rho_2(x) + \rho_2(x-a)\Big) \ , \qquad 2d < x
\end{aligned}$$

which solved together with (8.24) and using the continuity assumption leads to:

1. the two point correlation function reads:

$$\rho_2(x) = \frac{\rho^2}{1-\rho d} e^{-\frac{(x-d)\rho}{1-\rho d}} \ , \qquad d < x < 2d; \tag{8.25}$$

2. for every $k = 1, 2, \cdots$ if formula (8.23) holds for x in the interval $(kd, (k+1)d)$, then it holds also for x in the interval $((k+1)d, (k+2)d)$.

This concludes the proof. $\square$

It is known that in dimension one the correlation function are factorized in products of ρ_2. This is also valid for our solution, as stated by the following

Proposition 8.1.2 *The solution of (8.18) for $n \geq 2$ is*

$$\rho_n(q_1, \cdots, q_n) = \frac{1}{\rho^{n-2}} \prod_{j=1}^{n-1} \rho_2(q_j, q_{j+1}) \ . \tag{8.26}$$

Proof. We proceed by induction on n. For $n = 2$ we have an identity. Fix $n \geq 3$ and suppose (8.26) to be true for $n-1$. Then from (8.22) we have

$$\begin{aligned}
\rho_n(q_2 - d, q_2 \cdots, q_n) &= \frac{\rho}{1-\rho d} \rho_{n-1}(q_2, \cdots, q_n) \\
&= \frac{\rho^2}{1-\rho d} \frac{\prod_{j=2}^{n-1} \rho_2(q_j, q_{j+1})}{\rho^{n-2}} \ , \\
\frac{\partial \rho_n}{\partial q_1}(q_1, \cdots, q_n) &= R \rho_n(q_1, \cdots, q_n) \ , \qquad d < q_2 - q_1 < 2d \ , \\
\frac{\partial \rho_n}{\partial q_1}(q_1, \cdots, q_n) &= R \Big(\rho_n(q_1, \cdots, q_n) - \rho_n(q_1 + d, q_2, \cdots, q_n) \Big) \ , \qquad 2d < q_2 - q_1 \ .
\end{aligned}$$

Again this equation can be solved by induction on $k \geq 1$ for q_1 in the interval $(q_2 - (k+1)d, q_2 - kd)$, using the continuity assumption, thus leading to

$$\begin{aligned}
\rho_n(q_1, \cdots, q_n) &= \frac{1}{\rho^{n-2}} \prod_{j=2}^{n-1} \rho_2(q_j, q_{j+1}) \\
&\quad \times \rho \sum_{k=1}^{[(q_2-q_1)/d]} \Big(\frac{\rho}{1-\rho d} \Big)^k \frac{(q_2 - q_1 - kd)^{k-1}}{(k-1)!} e^{-\frac{(q_2-q_1-kd)\rho}{1-\rho d}} \ .
\end{aligned}$$

Using Proposition 8.1.1, this gives equation (8.26). □

Appendix A

Dynamics of hard spheres

In this appendix we state the properties of the dynamics of hard spheres that, together with Proposition 2.1.1 of Section 2.1, are used in our discussions.

First, we prove formula (2.15). We recall that the set $\Gamma_n^\dagger \cap \mathcal{K}_n$ is the maximal subset of the $n-$particle phase space over which our main result can be derived pointwise for all times. We do not know whether $\Gamma_n^* = \Gamma_n^\dagger$. However, we have

Lemma A.0.1 *For any $n \leq N$, the set $\Gamma_n \backslash \Gamma_n^\dagger$ has Lebesgue measure zero. Moreover, $\partial\Gamma_n \cap \left(\Gamma_n \setminus \Gamma_n^\dagger\right)$ is null with respect to the induced measure over $\partial\Gamma_n$.*

The induced measure over the boundary $d\sigma$ is given by Eq. (2.8). The lemma is a simple consequence of the existence of the dynamics over the full measure set Γ_n^*, stated in Proposition 2.1.1. Since we have no information on the structure of $\hat{\Gamma}_n$ nor its measurability properties, we will prove the lemma via abstract arguments.

Proof. It is sufficient to prove the assertion for any finite bound on the energy. A little abuse of notation will be used in what follows: we indicate with the usual symbols $\Gamma_n, \Gamma_n^*, \Gamma_n^\dagger$... the bounded sets corresponding to an energy of the system not larger than $E > 0$, and with $|\cdot|, |\cdot|^*$ respectively the restriction to the various sets of the Lebesgue measure and of the usual Lebesgue outer measure (that is the infimum, over all the possible coverings of a set built up with $n-$dimensional boxes, of the sum of the measures of such boxes). In the following we will use that the flow of the dynamics preserves also the outer measure, which can be easily deduced from the fact that it is an invertible measure preserving transformation (see [32], p. 651).

We abbreviate

$$\begin{aligned} Z_n^{(0)} &= \Gamma_n^* \setminus \Gamma_n^{\dagger(0)} , \\ Z_n &= \Gamma_n^* \setminus \Gamma_n^\dagger = \bigcup_{s\in\mathbb{R}} T_s^{(n)}(Z_n^{(0)}) . \end{aligned} \tag{A.1}$$

By Proposition 2.1.1, it is $|\Gamma_{n+k} \setminus \Gamma^*_{n+k}| = 0$ for any k, hence by the very definition $Z_n^{(0)}$ must be a null set. By the same reason, it suffices to prove that Z_n is a null set too. To do so, we use a contradiction argument: suppose that Z_n is *not* null; we will show that this implies the existence of a *not* null subset of $\Gamma_{n+k} \setminus \Gamma^*_{n+k}$ for some $k > 0$ (which is forbidden by Proposition 2.1.1).

For any $\underline{x}_n \in \Gamma^*_n, 1 \le k \le N - n$, call

$$B_k(\underline{x}_n) = \{\underline{y}_k \in \Gamma_k(\underline{x}_n) \text{ s.t. } (\underline{x}_n, \underline{y}_k) \in \Gamma_{n+k} \setminus \Gamma^*_{n+k}\}, \tag{A.2}$$

so that we can write $Z_n^{(0)} = \bigcup_{k=1}^{N-n} Z_{n,k}^{(0)}$,

$$Z_{n,k}^{(0)} = \{\underline{x}_n \in \Gamma^*_n \text{ s.t. } |B_k(\underline{x}_n)|^* > 0\}\ . \tag{A.3}$$

Given a function $\eta : Z_n^{(0)} \to (0, \infty)$, define also

$$Z_{n,k}^{(\eta)} = \bigcup_{\underline{x}_n \in Z_{n,k}^{(0)}} \ \bigcup_{s \in [-\eta(\underline{x}_n), \eta(\underline{x}_n)]} T_s^{(n)}(\underline{x}_n)\ , \qquad Z_n^{(\eta)} = \bigcup_{k=1}^{N-n} Z_{n,k}^{(\eta)}. \tag{A.4}$$

Observe that, in the assumption $|Z_n|^* \neq 0$, there exists necessarily a value of k such that,

$$\text{for any } \eta(\underline{x}_n) > 0, \qquad |Z_{n,k}^{(\eta)}|^* > 0\ . \tag{A.5}$$

Otherwise, take $\eta_0(\underline{x}_n) > 0$ for which $|Z_{n,k}^{(\eta_0)}|^* = 0$ for all k, and let ε_m be a sequence of positive numbers converging to zero: writing

$$\begin{aligned}
Z_n &= \bigcup_{m=1}^{\infty} \bigcup_{j \in \mathbb{Z}} \{T^{(n)}_{2j\eta_0(\underline{x}_n)}(\underline{x}_n), \underline{x}_n \in Z_n^{(\eta_0)} \text{ and } \eta_0(\underline{x}_n) > \varepsilon_m\} \\
&= \bigcup_{m=1}^{\infty} \bigcup_{j \in \mathbb{Z}} T^{(n)}_{2j\varepsilon_m} \left(Z_n^{(\varepsilon_m)} \bigcap \{T_s^{(n)}(\underline{x}_n),\ \text{with } \underline{x}_n \in Z_n^{(0)}, \eta_0(\underline{x}_n) > \varepsilon_m \text{ and } s \in \mathbb{R}\}\right)\ ,
\end{aligned}$$

we would get $|Z_n|^* = 0$ by subadditivity and preservation of the outer measure (the set in the argument of $T^{(n)}_{2j\varepsilon_m}$ is a subset of $Z_n^{(\eta_0)}$, hence it has outer measure zero).

From now on k indicates the variable for which the condition (A.5) holds. Given a function η, we can consider the following subsets:

$$\begin{aligned}
\tilde{B}_k(\underline{x}_n) &= \{\underline{y}_k \in B_k(\underline{x}_n) \mid \exists\ T_s^{(n+k)}(\underline{x}_n, \underline{y}_k)\ \forall s \in [-\eta(\underline{x}_n), \eta(\underline{x}_n)] \\
&\qquad \text{and } T_s^{(n+k)}(\underline{x}_n, \underline{y}_k) = (T_s^{(n)}(\underline{x}_n), T_s^{(k)}(\underline{y}_k))\}\ , \\
W_{n,k}^{(0)} &= \{(\underline{x}_n, \underline{y}_k) \text{ s.t. } \underline{x}_n \in Z_{n,k}^{(0)} \text{ and } \underline{y}_k \in \tilde{B}_k(\underline{x}_n)\}\ , \\
W_{n,k}^{(\eta)} &= \bigcup_{(\underline{x}_n, \underline{y}_k) \in W_{n,k}^{(0)}} \ \bigcup_{s \in [-\eta(\underline{x}_n), \eta(\underline{x}_n)]} T_s^{(n+k)}(\underline{x}_n, \underline{y}_k) \\
&\equiv \bigcup_{\underline{x}_n \in Z_{n,k}^{(0)}} \ \bigcup_{s \in [-\eta(\underline{x}_n), \eta(\underline{x}_n)]} \left(T_s^{(n)}(\underline{x}_n), T_s^{(k)}(\tilde{B}_k(\underline{x}_n))\right)\ .
\end{aligned} \tag{A.6}$$

By definition $W^{(0)}_{n,k} \subset \Gamma_{n+k} \setminus \Gamma^*_{n+k}$, and since $Z^{(0)}_n$ is null we have $|W^{(0)}_{n,k}| = 0$. Points of $W^{(0)}_{n,k}$ do not have well defined evolution for all times, but still the evolution exists up to times $\eta(\underline{x}_n)$, and this enables to define $W^{(\eta)}_{n,k}$. Notice now that for any $\underline{x}_n \in Z^{(0)}_n$

$$\begin{aligned}
|\tilde{B}_k(\underline{x}_n)|^* \geq |B_k(\underline{x}_n)|^* - |\{&\underline{y}_k \in \Gamma_k(\underline{x}_n) \text{ such that they experience} \\
&\text{at least one collision between themselves or with particles in } \underline{x}_n \\
&\text{or with the walls, when evolved with the } (n+k)\text{−th particle} \\
&\text{dynamics, within time } [-\eta(\underline{x}_n), \eta(\underline{x}_n)]\}|^* \\
&\geq |B_k(\underline{x}_n)|^* - O(\eta(\underline{x}_n)) \geq \frac{|B_k(\underline{x}_n)|^*}{2} > 0 \ ,
\end{aligned} \tag{A.7}$$

for $\eta(\underline{x}_n)$ sufficiently small (the bound with $O(\eta(\underline{x}_n))$ can be obtained by simple geometrical estimate; see for instance [3], p. 24-26, which can be easily adapted to our case).

Choose a function $\eta(\underline{x}_n)$ such that the above inequality holds. Then from the last line of Eq. (A.6), using (A.5), (A.7) and preservation of outer measure, we see that it must be

$$|W^{(\eta)}_{n,k}|^* > 0 \ . \tag{A.8}$$

Since $W^{(\eta)}_{n,k} \subset \Gamma_{n+k} \setminus \Gamma^*_{n+k}$, the contradiction is found. This proves that $\Gamma_n \setminus \Gamma^\dagger_n$ is a null set.

To prove the second assertion of the lemma, notice that a not σ_n−null set A_n over $\partial\Gamma_n$ in which the dynamics is everywhere well defined, spans a set of strictly posive outer measure over Γ_n through the operation $\bigcup_{s\in[0,T]}, T > 0$. In fact, the time return to $\partial\Gamma_n$ is $\tau(\underline{x}_n) > 0$ for almost all $\underline{x}_n$ of the set, and the Lebesgue measure over the subset of points of Γ_n whose previous collision was in $\partial\Gamma_n$ is $d\sigma_n dt$, t being the time elapsed after the collision ([32], [7]). Hence each "box" B_n of $\partial\Gamma_n$ spans at least a set of measure $\int_{B_n} d\sigma_n(\underline{x}_n)\tau(\underline{x}_n)$ in Γ_n. Conversely, each box of positive measure in Γ_n corresponds to a set of positive measure over $\partial\Gamma_n$: we refer to [32] for more details (see Lemma 3.1).Since $\bigcup_{s\in[0,T]}(Z_n \cap \partial\Gamma_n)$ is a subset of Z_n, which has been shown to be null, it follows that the set $Z_n \cap \partial\Gamma_n$ must be also null in the measure $d\sigma_n$ over $\partial\Gamma_n$. This, together with Proposition 2.1.1, completes the proof. □

Let us turn now our attention to the set $\mathcal{K}_n$. It is unclear whether $\mathcal{K}_n$ coincides with $\Gamma^\dagger_n$. In any case, what is relevant for our purposes is formula (2.16). To deduce it, we state another known feature of the hard sphere dynamics, which is related to the collision surfaces. Denote with $d\lambda$ the Lebesgue measure on $\mathbb{R}$.

Lemma A.0.2 *Given a set* $A \subset \Gamma_n$ *with* $|A| = 0$, *then* $T_t^{(n)}(\underline{x}_n) \notin A$ *for almost all* $(\underline{x}_n, t) \in \partial\Gamma_n \times \mathbb{R}$, *with respect to the product measure* $d\sigma_n \times d\lambda$.

The lemma can be easily deduced from the properties of the special flow representation discussed in [32], [7]. For a complete proof, we refer to [47] (Lemma 3.4). From Lemma A.0.2 it follows

Lemma A.0.3 *For any* $n \leq N$, *the set* $\Gamma_n \setminus \mathcal{K}_n$ *has Lebesgue measure zero.*

□

Appendix B

Proof of (5.13)

B.1 Case $m(\overline{\mathcal{D}}_{0;n+1}) = 0$

Consider a tree $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1}; [0,t]), \overline{\mathcal{D}} = (\underline{x}_{n+1}, \overline{\delta})$ and suppose $m(\overline{\mathcal{D}}_{0;n+1}) = 0$. We will prove the statement in this case first.

From (5.5) and (5.11) we see that

$$I(\overline{\mathcal{D}}) = \int_{\Gamma_1(\underline{x}_n)} dx_{n+1} \int_{\Delta_{\overline{\delta}}(\underline{x}_{n+1};[0,t])} d\hat{\delta} R(\underline{x}_{n+1}, \overline{\delta}, \hat{\delta}) \\ \equiv \int_{\Delta_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) \ , \tag{B.1}$$

where we called $\Delta_{n+1;\overline{\delta}}(\underline{x}_n; [0,t])$ the set of collision histories $\cup_{x_{n+1}\in\Gamma_1(\underline{x}_n)} \Delta_{\overline{\delta}}(\underline{x}_{n+1}; [0,t])$ (which is in one by one correspondence with the elements $\hat{\delta}' = (x_{n+1}, \hat{\delta})$), and $d\hat{\delta}' = dx_{n+1} d\hat{\delta}$ the measure over this set. By assumption (2.17) – see also (3.12) and discussion above –, R is a summable function over $\Delta_{n+1;\overline{\delta}}(\underline{x}_n; [0,t])$, and all the integrals can be interchanged freely.

Now introduce the subsets

$$\Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n; [0,t]) := \{\mathcal{D} \in \Delta_{n+1;\overline{\delta}}(\underline{x}_n; [0,t]) \text{ such that} \\ x_{n+1}(s; \mathcal{D}) = T^{(1)}_{-t+s+}(x_{n+1}) \ \forall s \in (t_{l^*(\overline{\delta})}, t)\} \ , \\ \Delta^{(k,i;+)}_{n+1;\overline{\delta}}(\underline{x}_n; [0,t]) := \{\mathcal{D} \in \Delta_{n+1;\overline{\delta}}(\underline{x}_n; [0,t]) \text{ such that} \\ x_{n+1}(s; \mathcal{D}) = T^{(1)}_{-t+s+}(x_{n+1}) \ \forall s \in (t^*, t) \ , \\ t^* \in (t_k, t_{k-1}) \text{ and } q_{n+1}(t^*; \mathcal{D}) - q_i(t^*; \mathcal{D}) = a\hat{w}^*, \\ |\hat{w}^*| = 1, \hat{w}^* \cdot (p_{n+1}(t^*; \mathcal{D}) - p_i(t^*; \mathcal{D})) > 0\} \ , \tag{B.2}$$

for $1 \leq k \leq l^*(\overline{\delta}), 1 \leq i \leq n+k-1$, where $l^*(\overline{\delta})$ is the variable defined in (5.7). In our assumption $l^*(\overline{\delta}) = m(\overline{\delta}) + 1$ (and $t_{l^*(\overline{\delta})} = 0$): we give the definition in this way because it will be useful to deal also with the more general cases. We remind the reader that the configuration of a particle in the evolution associated to a collision history is defined as the limit from the future of the flow of the dynamics; for example in (B.2) it is $q_{n+1}(t^*;\mathcal{D}) = T^{(1)}_{-t+t^*+}(x_{n+1})$, etc. Then

$$I(\overline{\mathcal{D}}) = \int_{\Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) \\ + \sum_{k=1}^{m(\overline{\delta})+1} \sum_{i=1}^{n+k-1} \int_{\Delta^{(k,i;+)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) \; . \tag{B.3}$$

Put, as usual, $\mathcal{D} = (\underline{x}_{n+1}, \overline{\delta}, \hat{\delta})$. In each term of the sums in the second line of (B.3) we can perform the change of variables

$$x_{n+1} \longrightarrow (t^*, \hat{p}^*, \hat{w}^*) \; , \tag{B.4}$$

where $t^*, \hat{w}^*$ are the variables introduced in the definition of the integration sets (B.2), and $\hat{p}^* := p_{n+1}(t^*;\mathcal{D}) \equiv p_{n+1}$. That is, t^* is the first time of collision of particle $n+1$ with the other particles of the collision history going backwards in time, particle i is the one colliding with $n+1$, and $\hat{w}^* := a^{-1}\left(q_{n+1}(t^*;\mathcal{D}) - q_i(t^*;\mathcal{D})\right)$. Then it is a simple exercise to see that the measure transforms as $d\hat{\delta}' = a^2 \hat{w}^* \cdot (\hat{p}^* - p_i(t^*;\mathcal{D})) dt^* d\hat{p}^* d\hat{w}^* d\hat{\delta}$ (see for instance the Appendix 4.B of [7]), where $p_i(\cdot)$ does not depend on the full $\mathcal{D} = (\underline{x}_{n+1}, \overline{\delta}, \hat{\delta})$ but just on $(t^*, \underline{x}_n, \overline{\delta}, \hat{\delta}) = (t^*, \overline{\mathcal{D}}_{/0;n+1}, \hat{\delta})$. Rename the dummy variables as $(t_l, \hat{p}_l, \hat{w}_l) \longrightarrow (t_{l+1}, \hat{p}_{l+1}, \hat{w}_{l+1})$ for $l = k, k+1, \cdots, m(\overline{\delta})$, and $(t^*, \hat{p}^*, \hat{w}^*) \longrightarrow (t_k, \hat{p}_k, \hat{w}_k)$, and call the new resulting set of variables

$$\hat{\gamma}_{k,i} := (t_1, \cdots, t_k, \cdots, t_{m(\overline{\delta})+1}, \hat{p}_1, \cdots, \hat{p}_k, \cdots, \hat{p}_{m(\overline{\delta})+1}, \hat{w}_1, \cdots, \hat{w}_k, \cdots, \hat{w}_{m(\overline{\delta})+1}) \; , \tag{B.5}$$

and also $d\hat{\gamma}_{k,i} := dt^* d\hat{p}^* d\hat{w}^* d\hat{\delta}$.

Consider now the tree defined by

$$\overline{\mathcal{G}}_{k,i} = (\underline{x}_n, \overline{\gamma}_{k,i}) := \overline{\mathcal{D}}_{/0;n+1} \circ_{k;i} \overline{\mathcal{D}}_{0;n+1} \in \overline{\Delta}(\underline{x}_n;[0,t]) \tag{B.6}$$

(in our case it is $\overline{\mathcal{D}}_{/0;n+1} = (\underline{x}_n, \overline{\delta})$, and $\overline{\mathcal{D}}_{0;n+1} = \overline{\mathcal{T}}$), and consider the collection of variables

$$\mathcal{G}_{k,i} := (\underline{x}_n, \overline{\gamma}_{k,i}, \hat{\gamma}_{k,i}) \; . \tag{B.7}$$

We shall see that, at least for a.a. $\underline{x}_n \in \Gamma^*_n$, the domain of integration of the new variables is the set of $\hat{\gamma}_{k,i}$ such that $\mathcal{G}_{k,i}$ is a collision history in $[0,t]$, with only one additional constraint on $\hat{w}_k$, which implies that particle created in the outcoming collision at time t_k would move freely in the future (since in (B.2) t^* is the *first* (backwards) time of collision of particle $n+1$ with the others).

First of all, it is clear that we can assign to $\mathcal{G}_{k,i}$ an evolution $\mathcal{E}_{\mathcal{G}_{k,i}}(s)$, $s \in [0,t]$, in the same way as we do for collision histories, and that this evolution is well defined in our domain of integration for almost all $\underline{x}_n \in \Gamma_n$ (the evolution coincides with $\mathcal{E}_{\mathcal{D}}$: just erase particle $n+1$ in the time interval (t^*, t)). Then, our integration region is defined as the set of $\hat{\gamma}_{k,i}$ such that: (i) $0 < t_{m(\overline{\gamma}_{k,i}) \equiv m(\overline{\delta})+1} < t_{m(\overline{\gamma}_{k,i})-1} < \cdots < t_1 < t$; (ii) $\hat{p}_1, \cdots, \hat{p}_{m(\overline{\gamma}_{k,i})} \in \mathbb{R}^3$; (iii) for $l = 1, \cdots, k-1, \hat{w}_l$ such that $\left(\underline{x}_{n+l-1}(t_l; \mathcal{G}_{k,i}), q_{j_l(\overline{\gamma}_{k,i})}(t_l; \mathcal{G}_{k,i}) + a\hat{w}_l, \hat{p}_l\right) \in \Gamma_{n+l}$; (iv) $\hat{w}_k \in \Omega^{(*)}_{i+}((\mathcal{G}_{k,i})_{/\hat{w}_k})$; (v) $\hat{w}_k$ is such that the clusters of particles of $\mathcal{G}_{k,i}$, $(1,2,\cdots,n,n+k), (1,2,\cdots,n+1,n+k), \cdots (1,2,\cdots,n+k-2,n+k)$ are respectively in $\Gamma^*_{n+1}, \Gamma^*_{n+2}, \cdots, \Gamma^*_{n+k-1}$, i.e. they do not run into singular configurations; (vi) for $l = k+1, \cdots, m(\overline{\gamma}_{k,i}), \hat{w}_l \in \Omega_{j_l(\overline{\gamma}_{k,i})}(\underline{x}_{n+l-1}(t_l; \mathcal{G}_{k,i}), \hat{p}_l)$. Now, restricting to $\underline{x}_n \in \Gamma^*_n$, consider the difference between the set defined by (i),...,(vi) and the set $\Delta^{(*)}_{\overline{\gamma}_{k,i}+}(\underline{x}_n; [0,t])$ defined in (5.14) (and equal to $\{\hat{\gamma}_{k,i}$ such that conditions (i), (ii), (iv), (vi) hold, and condition (iii) is modified by replacing Γ_{n+l} with Γ^*_{n+l}, that is by $\hat{w}_l \in \Omega_{j_l(\overline{\gamma}_{k,i})}(\underline{x}_{n+l-1}(t_l; \mathcal{G}_{k;i}), \hat{p}_l)$ for $l = 1, \cdots, k-1.\}$); this difference contains only values of $\hat{\gamma}_{k,i}$ such that some subcluster of particles of $(1, \cdots, n+k)$ run at some time into a singular configuration (and we can also notice that this singular configuration does not occur, in any case, along $\mathcal{E}_{\mathcal{G}_{k,i}}(s)$ for $s \in [0,t]$). Hence, *for almost all* $\underline{x}_n \in \Gamma^*_n$ the integral in $d\hat{\gamma}_{k,i}$ over the difference set must give zero contribution: otherwise we could find, in the phase space of such cluster of particles, a set with Lebesgue measure different from zero over which the dynamics is not well defined (contradiction with [3], [32]). We do not give a formal proof of the last statement (which is not difficult to believe): this can be found in [47] (see Lemma 6.2 of that work).

In conclusion, noticing that, after the above renaming of the variables,

$$p_i(t^*; \overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}) = p_i(t_k; \mathcal{G}_{k,i})$$

and

$$a^2 \hat{w}^* \cdot (\hat{p}^* - p_i(t^*; \overline{\mathcal{D}}_{/0;n+1}, \hat{\delta})) R(\underline{x}_n, x_{n+1}(t^*, \hat{p}^*, \hat{w}^*), \overline{\delta}, \hat{\delta}) \longrightarrow R(\mathcal{G}_{k,i}) \ , \tag{B.8}$$

we have obtained

$$\int_{\Delta^{(k,i;+)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) = \int_{\Delta^{(*)}_{\overline{\gamma}_{k,i}+}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i} R(\underline{x}_n, \overline{\gamma}_{k,i}, \hat{\gamma}_{k,i}) \tag{B.9}$$

almost everywhere in Γ_n.

Now we want to deal with the term in the first line of (B.3). For almost all $\underline{x}_n \in \Gamma_n^*$ the integration region in the term considered can be rewritten as

$$\Big\{\hat{\delta}' = (x_{n+1}, \hat{\delta}) \text{ such that } (\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}) \in \Delta_{\overline{\delta}}(\underline{x}_n; [0,t]) \text{ and} \qquad \text{(B.10)}$$
$$\Big(\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(s), T^{(1)}_{-t+s+}(x_{n+1})\Big) \in \Gamma_{\mathcal{N}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(s)+1} \ \forall s \in (0,t)\Big\} \ ;$$

in fact we can notice, as done just above, that the error term is an integral over a region of zero measure, corresponding to singular trajectories. In the region (B.10) the dependence of the integrand on the variable x_{n+1} is concentrated on the correlation function, since the particles of the evolution appearing in the definition of the set evolve independently of x_{n+1} in our assumption $m(\overline{\mathcal{D}}_{0;n+1}) = 0$. Explicitly,

$$R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) = W\left(\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}\right) \rho_{n+1+m(\overline{\delta})}\left(T^{(1)}_{-t+}(x_{n+1}), \mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right) \qquad \text{(B.11)}$$

(here we used the symmetry of the correlation functions).

Hence by making the change of variables

$$x_{n+1} \longrightarrow x'_{n+1} = T^{(1)}_{-t+}(x_{n+1}) \qquad \text{(B.12)}$$

we obtain the integration over

$$\Big\{\hat{\delta}'' = (x'_{n+1}, \hat{\delta}) \text{ such that } (\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}) \in \Delta_{\overline{\delta}}(\underline{x}_n; [0,t]) \text{ and} \qquad \text{(B.13)}$$
$$\Big(\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(s), T^{(1)}_{s-}(x'_{n+1})\Big) \in \Gamma_{\mathcal{N}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(s)+1} \ \forall s \in (0,t)\Big\} \ ,$$

in $d\hat{\delta}''$, of the function

$$W\left(\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}\right) \rho_{n+1+m(\overline{\delta})}\left(x'_{n+1}, \mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right) \ . \qquad \text{(B.14)}$$

We want to complete now the integral in order to obtain the function $\rho_{n+m(\overline{\delta})}$. This can be done extending the integration to the full set

$$\Big\{\hat{\delta}'' = (x'_{n+1}, \hat{\delta}) \text{ such that } (\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}) \in \Delta_{\overline{\delta}}(\underline{x}_n; [0,t]) \qquad \text{(B.15)}$$
$$\text{and } x'_{n+1} \in \Gamma_{n+m(\overline{\delta})}(\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0))\Big\} \ .$$

The integral in $d\hat{\delta}''$, over the region (B.15), of function (B.14) gives, after ordering the integrations,

$$\int_{\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta} W\left(\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}\right) \int_{\Gamma_{n+m(\overline{\delta})}(\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0))} dx'_{n+1} \qquad \text{(B.16)}$$
$$\cdot \rho_{n+1+m(\overline{\delta})}\left(x'_{n+1}, \mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right)$$
$$= (N-n-m(\overline{\delta})) \int_{\Delta_{\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta} W\left(\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}\right) \rho_{n+m(\overline{\delta})}\left(\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right)$$
$$= (N-n-m(\overline{\delta}))V(\overline{\mathcal{D}}_{/0;n+1}) \ .$$

Subtracting the error term, we have obtained

$$
\begin{aligned}
&\int_{\Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) = (N - n - m(\overline{\delta}))V(\overline{\mathcal{D}}_{/0;n+1}) \\
&- \sum_{k=1}^{m(\overline{\delta})+1} \sum_{i=1}^{n+k-1} \int_{\Delta^{(k,i;-)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}'' W\left(\overline{\mathcal{D}}_{/0;n+1}, \hat{\delta}\right) \\
&\quad \cdot \rho_{n+1+m(\overline{\delta})}\left(x'_{n+1}, \mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right) \qquad \text{(B.17)}
\end{aligned}
$$

for almost all $\underline{x}_n \in \Gamma_n$, where

$$
\begin{aligned}
\Delta^{(k,i;-)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t]) := \Big\{ &\hat{\delta}'' = (x'_{n+1}, \hat{\delta}) \text{ such that } (\underline{x}_n, \overline{\delta}, \hat{\delta}) \in \Delta_{\overline{\delta}}(\underline{x}_n;[0,t]) \text{ and} \\
&\left(\mathcal{E}_{(\underline{x}_n,\overline{\delta},\hat{\delta})}(s), T^{(1)}_{s-}(x'_{n+1})\right) \in \Gamma_{\mathcal{N}_{(\underline{x}_n,\overline{\delta},\hat{\delta})}(s)+1} \ \forall s \in (0,t^*), \\
&t^* \in (t_k, t_{k-1}), \text{ and } (T^{(1)}_{s-}(x'_{n+1}))_q - q_i(t^*; \underline{x}_n, \overline{\delta}, \hat{\delta}) = a\hat{w}^*, \\
&|\hat{w}^*| = 1, \hat{w}^* \cdot ((T^{(1)}_{s-}(x'_{n+1}))_p - p_i(t^*; \underline{x}_n, \overline{\delta}, \hat{\delta})) < 0 \Big\}. \qquad \text{(B.18)}
\end{aligned}
$$

In expression (B.17) we have decomposed the error term in a sum of integrals, where labels k and i describe between which nodes and with which particle of $\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}$ occurs the first collision, moving *forward* in time, of the external particle with initial configuration x'_{n+1} at time 0. Once again to write (B.17) we removed sets of zero measure (i.e. points $x'_{n+1} \in \Gamma_1 \setminus \Gamma_1^*$).

We can treat the terms in the second line of (B.17) as we did for those in (B.3). In this case we perform a change of variable

$$
x'_{n+1} \longrightarrow (t^*, \hat{p}^*, \hat{w}^*), \qquad \text{(B.19)}
$$

where $t^*, \hat{p}^*$ are the variables introduced in the definition (B.18) and $\hat{p}^* := p'_{n+1}$. The measure transforms as $d\hat{\delta}'' = -a^2 \hat{w}^* \cdot (\hat{p}^* - p_i(t^*; \underline{x}_n, \overline{\delta}, \hat{\delta}))dt^* d\hat{p}^* d\hat{w}^* d\hat{\delta}$. We rename the dummy variables as $(t_l, \hat{p}_l, \hat{w}_l) \longrightarrow (t_{l+1}, \hat{p}_{l+1}, \hat{w}_{l+1})$ for $l = k, k+1, \cdots, m(\overline{\delta})$, and $(t^*, \hat{p}^*, \hat{w}^*) \longrightarrow (t_k, \hat{p}_k, \hat{w}_k)$, and we introduce the same notations of (B.5), (B.6), (B.7). We can assign to $\mathcal{G}_{k,i}$ an evolution $\mathcal{E}_{\mathcal{G}_{k,i}}(s), s \in [0,t]$, which is well defined in our domain of integration for all $\underline{x}_n \in \Gamma_n^*$, and that is obtained by adding to $\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}$ the free flow of x'_{n+1} in the time interval $[0, t_k]$). Moreover, for almost all $\underline{x}_n \in \Gamma_n^*$, the domain of integration of the new variables is the set of $\hat{\gamma}_{k,i}$ such that $\mathcal{G}_{k,i}$ is a collision history in $[0,t]$, with only one additional constraint on $\hat{w}_k$, which implies that particle created in the incoming collision at time t_k moves freely in the past (since in (B.18) t^* is the *first* (forward) time of collision of the particle starting in x'_{n+1} with one of the others); this is so by forgetting, as usual, the zero measure sets in which some cluster of particles of $\mathcal{G}_{k,i}$ run at some time into a singular configuration. This means that, making use of the definitions (5.14), (5.9), and rewriting the integrand with the notations introduced,

$$-\int_{\Delta^{(k,i;-)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}''W\left(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta}\right)\rho_{n+1+m(\overline{\delta})}\left(x'_{n+1},\mathcal{E}_{(\overline{\mathcal{D}}_{/0;n+1},\hat{\delta})}(0)\right)$$
$$= +\int_{\Delta^{(*)}_{\overline{\gamma}_{k,i}-}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i}R(\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i}) \tag{B.20}$$

almost everywhere in Γ_n.

This last equation, together with (B.17), (B.3) and (B.9), gives (5.13).

B.2 Case $m(\overline{\mathcal{D}}_{0;n+1}) > 0$

Let us consider a tree $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_{n+1};[0,t]), \overline{\mathcal{D}} = (\underline{x}_{n+1},\overline{\delta})$, with $m(\overline{\mathcal{D}}_{0;n+1}) > 0$. This case is very similar to the previous one and it is discussed essentially in the same way, with the only difference that the role played by time $t_{m(\overline{\delta})+1} \equiv 0$ is now played by $t_{l^*(\overline{\delta})} \equiv t_{q_1^{(n+1)}(\overline{\delta})}$ – see (5.6), (5.7) (through all this section l^* and $\underline{q}^{(n+1)}$ will indicate the values associated to $\overline{\delta}$ defined by (5.6) and (5.7)).

In particular, the analysis from (B.1) to (B.9) is exactly the same once we restrict to l^* the sum over k in (B.3), and substitute (B.6) with

$$\overline{\mathcal{G}}_{k,i} = (\underline{x}_n,\overline{\gamma}_{k,i}) := \overline{\mathcal{D}}_{/0;n+1}\circ_{k,\underline{q}_+^{(n+1)};i}\overline{\mathcal{D}}_{0;n+1} \in \overline{\Delta}(\underline{x}_n;[0,t])\ . \tag{B.21}$$

Hence we have again

$$I(\overline{\mathcal{D}}) = \int_{\Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}'R(\underline{x}_n,x_{n+1},\overline{\delta},\hat{\delta}) \tag{B.22}$$
$$+\sum_{k=1}^{l^*}\sum_{i=1}^{n+k-1}\int_{\Delta^{(*)}_{\overline{\gamma}_{k,i}+}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i}R(\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i})$$

almost everywhere in Γ_n. Of course now $\overline{\mathcal{D}}_{/0;n+1} \neq (\underline{x}_n,\overline{\delta})$, and $\overline{\mathcal{D}}_{0;n+1} \neq \overline{\mathcal{T}}$, but they have a more complicated structure depending on the labels attached to the nodes on the root line of the tree $\overline{\mathcal{D}}$.

Call $\mathcal{D}^{(*)}_+$ the collection of variables obtained from the collision history $\mathcal{D} = (\underline{x}_n,x_{n+1},\overline{\delta},\hat{\delta})$ by *depriving* it of x_{n+1} and of the variables associated to the nodes with ordering number larger than l^*-1, and substituting $m(\overline{\delta})$ with l^*-1. With the usual notations (Eq. (3.3) and (5.10)),

$$\mathcal{D}^{(*)}_+ = (\underline{x}_n,l^*-1,j_1,\cdots,j_{l^*-1},t_1,\cdots,t_{l^*-1},\hat{p}_1,\cdots,\hat{p}_{l^*-1},\hat{w}_1,\cdots,\hat{w}_{l^*-1})\ . \tag{B.23}$$

Then, for almost all $\underline{x}_{n+1} \in \Gamma_{n+1}$ such that $\mathcal{D} \in \Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])$, it is also $\mathcal{D}^{(*)}_+ \in \Delta(\underline{x}_n;[t_{l^*},t])$: that is the same collision history restricted to the time interval

$(t_{l^*}, t]$, and deprived of particle $n+1$. For these values of $\underline{x}_{n+1}$, putting $x'_{n+1} = T^{(1)}_{-t+t_{l^*}+}(x_{n+1})$, we may define also a collision history with time span $[0, t_{l^*}]$ by

$$\mathcal{D}^{(*)}_- = \Big(\mathcal{E}_{\mathcal{D}^{(*)}_+}(t_{l^*}), x'_{n+1}, q'_{n+1} + a\hat{w}_{l^*}, \hat{p}_{l^*}, m(\overline{\delta}) - l^*, \tag{B.24}$$
$$j_{l^*+1}, \cdots, j_{m(\overline{\delta})}, t_{l^*+1}, \cdots, t_{m(\overline{\delta})}, \hat{p}_{l^*+1}, \cdots, \hat{p}_{m(\overline{\delta})}, \hat{w}_{l^*+1}, \cdots, \hat{w}_{m(\overline{\delta})}\Big) .$$

This will belong to $\Delta_{\mathcal{N}_{\mathcal{D}^{(*)}_+(t_{l^*})}+2}(\mathcal{E}_{\mathcal{D}^{(*)}_+}(t_{l^*}), x'_{n+1}, q'_{n+1} + a\hat{w}_{l^*}, \hat{p}_{l^*}; [0, t_{l^*}])$.

We can rewrite the integration region on the first line of (B.22) as the set of values of $\hat{\delta}'$ such that $x_{n+1}(s; \mathcal{D}) = T^{(1)}_{-t+s+}(x_{n+1})$ $\forall s \in (t_{l^*}, t)$, $\mathcal{D}^{(*)}_+ \in \Delta(\underline{x}_n; [t_{l^*}, t])$ and $\mathcal{D}^{(*)}_- \in \Delta_{\mathcal{N}_{\mathcal{D}^{(*)}_+(t_{l^*})}+2}(\mathcal{E}_{\mathcal{D}^{(*)}_+}(t_{l^*}), x'_{n+1}, q'_{n+1} + a\hat{w}_{l^*}, \hat{p}_{l^*}; [0, t_{l^*}])$ (we are just discarding a zero measure set for almost all $\underline{x}_n \in \Gamma_n$). After that, we perform the change of variables

$$x_{n+1} \longrightarrow x'_{n+1} = T^{(1)}_{-t+t_{l^*}+}(x_{n+1}) . \tag{B.25}$$

We obtain

$$\int_{\Delta^{(0)}_{n+1;\overline{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \overline{\delta}, \hat{\delta}) \tag{B.26}$$
$$= \int_{\mathcal{A}} d\hat{\delta}'' \left(\prod_{r=1}^{l^*-1} W_r(\mathcal{D}^{(*)}_+)\right) a^2 \hat{w}_{l^*} \cdot (\hat{p}_{l^*} - p'_{n+1}) R(\mathcal{D}^{(*)}_-) ,$$

where $\mathcal{A}$ is a short notation for

$$\mathcal{A} := \Big\{\hat{\delta}'' = (x'_{n+1}, \hat{\delta}) \text{ such that } \mathcal{D}^{(*)}_+ \in \Delta(\underline{x}_n; [t_{l^*}, t]) , \tag{B.27}$$
$$\mathcal{D}^{(*)}_- \in \Delta_{\mathcal{N}_{\mathcal{D}^{(*)}_+(t_{l^*})}+2}(\mathcal{E}_{\mathcal{D}^{(*)}_+}(t_{l^*}), x'_{n+1}, q'_{n+1} + a\hat{w}_{l^*}, \hat{p}_{l^*}; [0, t_{l^*}]) ,$$
$$\text{and } \left(\mathcal{E}_{\mathcal{D}^{(*)}_+}(s), T^{(1)}_{-t_{l^*}+s-}(x'_{n+1})\right) \in \Gamma_{\mathcal{N}_{\mathcal{D}^{(*)}_+}(s)+1} \;\forall s \in (t_{l^*}, t)\Big\} .$$

Observe that the values of $\hat{w}_{l^*}, \hat{p}_{l^*}$ in $\hat{\delta}$ associated to the particle colliding, at time t_{l^*}, with the one in x'_{n+1} in the evolution $\mathcal{D}^{(*)}_-$, describe both outgoing and ingoing collisions: we will strongly use this fact at the end of the proof.

Extend now the integral to the integration region

$$\mathcal{B} := \Big\{\hat{\delta}'' = (x'_{n+1}, \hat{\delta}) \text{ such that } \mathcal{D}^{(*)}_+ \in \Delta(\underline{x}_n; [t_{l^*}, t]) , \tag{B.28}$$
$$\mathcal{D}^{(*)}_- \in \Delta_{\mathcal{N}_{\mathcal{D}^{(*)}_+(t_{l^*})}+2}(\mathcal{E}_{\mathcal{D}^{(*)}_+}(t_{l^*}), x'_{n+1}, q'_{n+1} + a\hat{w}_{l^*}, \hat{p}_{l^*}; [0, t_{l^*}])\Big\} ,$$

and notice that the error term is an integral over the set of variables such that, for some $1 \leq k \leq l^*, 1 \leq i \leq n+k-1, t^* \in (t_k, t_{k-1}), \hat{w}^* \in S^1$, it occurs that

$$\left(\mathcal{E}_{\mathcal{D}^{(*)}_+}(s), T^{(1)}_{-t_{l^*}+s-}(x'_{n+1})\right) \in \Gamma_{\mathcal{N}_{\mathcal{D}^{(*)}_+}(s)+1} \tag{B.29}$$

for all $s \in (t_{l^*}, t^*)$, and

$$
\begin{aligned}
&(T^{(1)}_{-t_{l^*}+t^*-}(x'_{n+1}))_q - q_i(t^*; \mathcal{D}^{(*)}_+) = a\hat{w}^* \, , \\
&\hat{w}^* \cdot \Big((T^{(1)}_{-t_{l^*}+t^*-}(x'_{n+1}))_p - p_i(t^*; \mathcal{D}^{(*)}_+) \Big) \neq 0 \qquad (\text{hence} < 0)
\end{aligned}
\tag{B.30}
$$

(particle i is now identified ordering, in the usual way, the particles of $\mathcal{D}^{(*)}_+ \in \Delta(\underline{x}_n; [t_{l^*}, t]))$.

Then in $\mathcal{B} \setminus \mathcal{A}$, calling $\hat{p}^* = (T^{(1)}_{-t_{l^*(\bar{\delta})}+t^*-}(x'_{n+1}))_p$, we can associate to x'_{n+1} the triple $(t^*, \hat{p}^*, \hat{w}^*)$. Adding to $\hat{\delta}$ the triple $(t^*, \hat{p}^*, \hat{w}^*)$ and renaming the variables as explained before (B.5), we obtain a collection $\hat{\gamma}_{k,i}$ defined as in (B.5). This, together with (B.7) and (B.21), defines a collision history associated to the tree $\bar{\mathcal{G}}_{k,i}$, as soon as the corresponding clusters of particles do not run into a singular configuration. Clearly, in this case it must be $\mathcal{G}_{k,i} \in \Delta^{(*)}_{\bar{\gamma}_{k,i}-}(\underline{x}_n; [0, t])$. Moreover, $d\hat{\delta}'' = -a^2 \hat{w}_k \cdot (\hat{p}_k - p_i(t_k; \mathcal{G}_{k,i})) d\hat{\gamma}_{k,i}$ (where $t_k, \hat{p}_k, \hat{w}_k$ are now the elements in $\mathcal{G}_{k,i}$). By performing this change of variables and erasing sets of zero measure, we see that Eq. (B.26) becomes

$$
\begin{aligned}
&\int_{\Delta^{(0)}_{n+1;\bar{\delta}}(\underline{x}_n;[0,t])} d\hat{\delta}' R(\underline{x}_n, x_{n+1}, \bar{\delta}, \hat{\delta}) = \int_{\mathcal{B}} d\hat{\delta}'' \left(\prod_{r=1}^{l^*-1} W_r(\mathcal{D}^{(*)}_+) \right) \\
&\quad \cdot a^2 \hat{w}_{l^*} \cdot (\hat{p}_{l^*} - p'_{n+1}) R(\mathcal{D}^{(*)}_-) \\
&\quad - \sum_{k=1}^{l^*(\bar{\delta})} \sum_{i=1}^{n+k-1} \int_{\Delta^{(*)}_{\bar{\gamma}_{k,i}-}(\underline{x}_n;[0,t])} d\hat{\gamma}_{k,i} R(\underline{x}_n, \bar{\gamma}_{k,i}, \hat{\gamma}_{k,i})
\end{aligned}
\tag{B.31}
$$

for almost all $\underline{x}_n \in \Gamma_n$.

Furthermore, the first term in the right hand side of the above equation is *equal to zero* for almost every $\underline{x}_n \in \Gamma_n$. In fact, there exists an involution that associates to each element $\hat{\delta}''_1$ of $\mathcal{B}$ another element $\hat{\delta}''_2$ of the same set in such a way that the corresponding values of the integrand function have the same modulus and opposite sign. This involution is given by the collision rule applied to the two particles colliding at time t_{l^*} in $\mathcal{D}^{(*)}_-$, as explained in what follows.

Given $\hat{\delta}''_1 = (y_1, \hat{\delta}_1)$, $y_1 = ((y_1)_q, (y_1)_p)$,

$$
\hat{\delta}_1 = (t_1, \cdots, t_{l^*}, \cdots, t_{m(\bar{\delta})}, \hat{p}_1, \cdots, \hat{p}_{l^*}, \cdots, \hat{p}_{m(\bar{\delta})}, \hat{w}_1, \cdots, \hat{w}_{l^*}, \cdots, \hat{w}_{m(\bar{\delta})}) \, ,
\tag{B.32}
$$

by definition of $\mathcal{D}^{(*)}_-$ it follows that in its starting time t_{l^*} we have always a particle in the configuration $((y_1)_q + a\hat{w}_{l^*}, \hat{p}_{l^*})$. We put $\hat{\delta}''_2 = (y_2, \hat{\delta}_2)$ with $(y_2)_q = (y_1)_q$, $(y_2)_p = (y_1)_p + \hat{w}_{l^*}[\hat{w}_{l^*} \cdot (\hat{p}_{l^*} - (y_1)_p)]$, and $\hat{\delta}_2$ equal to $\hat{\delta}_1$ except for the component $\hat{p}_{l^*}$ which is replaced by $\hat{p}'_{l^*} = \hat{p}_{l^*} - \hat{w}_{l^*}[\hat{w}_{l^*} \cdot (\hat{p}_{l^*} - (y_1)_p)]$. The element $\hat{\delta}''_2$ will belong to $\mathcal{B}$. Looking at the integrand function, notice that the transformation $\hat{\delta}_1'' \longrightarrow \hat{\delta}_2''$ leaves unchanged the value of $R(\mathcal{D}_-^{(*)})$, as well as the value of the functions $W_r(\mathcal{D}_+^{(*)})$ for all $1 \leq r \leq l^* - 1$, but transforms $a^2 \hat{w}_{l^*} \cdot (\hat{p}_{l^*} - (y_1)_p)$ into $a^2 \hat{w}_{l^*} \cdot (\hat{p}'_{l^*} - (y_2)_p) = -a^2 \hat{w}_{l^*} \cdot (\hat{p}_{l^*} - (y_1)_p)$. Hence the integrand function changes its sign.

Hence, equations (B.22) and (B.31) give the result. $\square$

Appendix C

Proof of Lemma 5.2.1

Fix $\underline{x}_n \in \Gamma_n^*$, and look at elements $\hat{\gamma}_{k,i} \in \Delta_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t]) \setminus \Delta^{(*)}_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t])$. By definition (5.9) and using the notations (B.5) and (B.7), we have two cases:

1. $\hat{w}_k \in \Omega_{j_k(\overline{\gamma}_{k,i})+}(\underline{x}_{n+k-1}(t_k;\mathcal{G}_{k,i}),\hat{p}_k)$, and there exists $1 \leq k' \leq k$ and $1 \leq i' \leq n+k'-1$ such that for some time $t^* \in (t_{k'},t_{k'-1}), \hat{w}^* \in S^2$, it is

$$\begin{aligned}
&\left(\mathcal{E}_{\mathcal{G}_{k,i}}(s), T^{(1)}_{-t_k+s-}\left(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k\right)\right) \in \Gamma_{\mathcal{N}_{\mathcal{G}_{k,i}}(s)+1}\ \forall s \in (t_k,t^*)\ ,\\
&\left(T^{(1)}_{-t_k+t^*-}(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k)\right)_q - q_{i'}(t^*;\mathcal{G}_{k,i}) = a\hat{w}^*\ ,\\
&\hat{w}^*\cdot\left(\left(T^{(1)}_{-t_k+t^*-}(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k)\right)_p - p_{i'}(t^*;\mathcal{G}_{k,i})\right) < 0\ ;
\end{aligned} \tag{C.1}$$

2. $\hat{w}_k \in \Omega_{j_k(\overline{\gamma}_{k,i})-}(\underline{x}_{n+k-1}(t_k;\mathcal{G}_{k,i}),\hat{p}_k)$, and there exists $k+1 \leq k' \leq l^*$ and $1 \leq i' \leq n+k'-1$ such that for some time $t^* \in (t_{k'},t_{k'-1}), \hat{w}^* \in S^2$, it is

$$\begin{aligned}
&\left((\mathcal{E}_{\mathcal{G}_{k,i}})_{/k}(s), T^{(1)}_{-t_k+s+}\left(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k\right)\right) \in \Gamma_{\mathcal{N}_{\mathcal{G}_{k,i}}(s)}\forall s \in (t^*,t_k)\ ,\\
&\left(T^{(1)}_{-t_k+t^*+}(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k)\right)_q - q_{i'}(t^*;\mathcal{G}_{k,i}) = a\hat{w}^*\ ,\\
&\hat{w}^*\cdot\left(\left(T^{(1)}_{-t_k+t^*+}(q_{j_k(\overline{\gamma}_{k,i})}(t_k;\mathcal{G}_{k,i})+a\hat{w}_k,\hat{p}_k)\right)_p - p_{i'}(t^*;\mathcal{G}_{k,i})\right) > 0\ .
\end{aligned} \tag{C.2}$$

Denote $\mathcal{R}_+$ and $\mathcal{R}_-$ the sets of triples $(k,i,\hat{\gamma}_{k,i})$ with $1 \leq k \leq l^*$, $1 \leq i \leq n+k-1$, and $\hat{\gamma}_{k,i} \in \Delta_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t]) \setminus \Delta^{(*)}_{\overline{\gamma}_{k,i}}(\underline{x}_n;[0,t])$ satisfying respectively property 1 and property 2 of the list above. Introduce a measure $d\varrho$ over $\mathcal{R}_+ \cup \mathcal{R}_-$ as the counting measure with respect to k,i and the Lebesgue measure with respect to $\hat{\gamma}_{k,i}$, and rewrite the left hand side of (5.15) in the short notation

$$\int_{\mathcal{R}_+} d\varrho R(\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i}) + \int_{\mathcal{R}_-} d\varrho R(\underline{x}_n,\overline{\gamma}_{k,i},\hat{\gamma}_{k,i})\ . \tag{C.3}$$

We may define a transformation J over almost all $\mathcal{R}_+$ as

$$J(k,i,\hat{\gamma}_{k,i}) = (k',i',\hat{\eta}_{k',i'})\ , \tag{C.4}$$

where k', i' are defined in point 1 of the list above, and

$$\hat{\eta}_{k',i'} = (t'_1, \cdots, t'_{m(\overline{\gamma}_{k,i})}, \hat{p}'_1, \cdots, \hat{p}'_{m(\overline{\gamma}_{k,i})}, \hat{w}'_1, \cdots, \hat{w}'_{m(\overline{\gamma}_{k,i})}) \tag{C.5}$$

is constructed from the collection of variables $\hat{\gamma}_{k,i}$, substituting the elements $(t_k, \hat{w}_k)$ with $(t^*, \hat{w}^*)$ (defined in point 1 of the list above), and reordering the components to obtain the usual decreasing sequence of times. Notice that $(\underline{x}_n, \overline{\gamma}_{k',i'})$ is the tree that is obtained from $\overline{\gamma}_{k,i}$ pruning the subtree generated in the $k-$th node and reattaching it to the line representing particle i', in such a way that a new node with ordering number k' is created, and that all the other nodes maintain the same mutual ordering. Then, it is clear that $\hat{\eta}_{k',i'}$ is in $\Delta_{\overline{\gamma}_{k',i'}}(\underline{x}_n; [0,t])$ as soon as all the clusters of particles associated to it do not run into singular configurations for all times. This is true for almost all $\hat{\gamma}_{k,i}$, at least for almost every $\underline{x}_n \in \Gamma^*_n$. Moreover in this case, by construction, $\hat{\eta}_{k',i'}$ is in $\Delta_{\overline{\gamma}_{k',i'}}(\underline{x}_n; [0,t]) \setminus \Delta^{(*)}_{\overline{\gamma}_{k',i'}}(\underline{x}_n; [0,t])$, and it satisfies property 2 in the list above, i.e. $(k', i', \hat{\eta}_{k',i'})$ is in $\mathcal{R}_-$. Hence

$$J : \mathcal{R}^*_+ \longrightarrow \mathcal{R}_- \tag{C.6}$$

where $\mathcal{R}^*_+ \subset \mathcal{R}_+$ and $\mathcal{R}_+ \setminus \mathcal{R}^*_+$ has zero measure (for almost all $\underline{x}_n \in \Gamma^*_n$). Furthermore, the inverse function J^{-1} is defined over almost all $\mathcal{R}_-$ in a natural way. In particular, $\mathcal{R}^*_- = J(\mathcal{R}^*_+) \subset \mathcal{R}_-$, $\mathcal{R}_- \setminus \mathcal{R}^*_-$ being a zero measure subset.

After substituting $\mathcal{R}_+$ and $\mathcal{R}_-$ in (C.3) with $\mathcal{R}^*_+$ and $\mathcal{R}^*_-$, we perform the change of variables $(k, i, \hat{\gamma}_{k,i}) \longrightarrow J(k, i, \hat{\gamma}_{k,i})$ in the first integral. The function

$$\prod_{\substack{r=1 \\ r\neq k}}^{m(\overline{\gamma}_{k,i})} W_r(\mathcal{G}_{k,i}) \rho_{n+m(\overline{\gamma}_{k,i})}(\underline{x}_{n+m(\overline{\gamma}_{k,i})}(\mathcal{G}_{k,i})) \tag{C.7}$$

is invariant under this transformation, while the measure transforms as

$$d\hat{\gamma}_{k,i} W_k(\underline{x}_n, \overline{\gamma}_{k,i}, \hat{\gamma}_{k,i}) = -d\hat{\eta}_{k',i'} W_{k'}(\underline{x}_n, \overline{\gamma}_{k',i'}, d\hat{\eta}_{k',i'}) \; . \tag{C.8}$$

Therefore, the two terms in formula (C.3) cancel each other. □

Appendix D

Continuity properties

In this appendix we prove some property needed in the discussion of Section 4.1. We always assume to work with an initial measure P with density $f_N \in \mathcal{L}_N$; Liouville equation and correlation functions are defined by (4.5), which is assumed to hold, for simplicity, on the whole set $\Gamma_n^{\dagger(+)}$ (defined as in (4.4)). The value of trees is defined by (3.10).

The following mild continuity property of the correlation functions can be derived with no need of additional assumptions on the initial measure (and, as expected, $V(\overline{\mathcal{D}})$ inherits the same property as a function of $(\underline{x}_n, t)$).

Lemma D.0.1 *For all $\underline{x}_n \in \Gamma_n^{\dagger(+)}$, the functions of time*

$$\begin{aligned} &t \longrightarrow \rho_n(T_t^{(n)}(\underline{x}_n), t) \ , \\ &t \longrightarrow V(\overline{\mathcal{D}})(T_t^{(n)}(\underline{x}_n), t) \end{aligned} \tag{D.1}$$

with $\overline{\mathcal{D}} \in \overline{\Delta}(\underline{x}_n; [0, t])$, are continuous for all $t > 0$, that is

$$\begin{aligned} &\lim_{\varepsilon \to 0^+} \rho_n(T_{+\varepsilon}^{(n)}(\underline{x}_n), t + \varepsilon) = \lim_{\varepsilon \to 0^+} \rho_n(T_{-\varepsilon}^{(n)}(\underline{x}_n), t - \varepsilon) \ , \\ &\lim_{\varepsilon \to 0^+} V(\overline{\mathcal{D}})(T_{+\varepsilon}^{(n)}(\underline{x}_n), t + \varepsilon) = \lim_{\varepsilon \to 0^+} V(\overline{\mathcal{D}})(T_{-\varepsilon}^{(n)}(\underline{x}_n), t - \varepsilon) \end{aligned} \tag{D.2}$$

hold for all $t > 0$ and all $\underline{x}_n \in \Gamma_n^\dagger$. In particular, Eq. (D.2) is true for all $t > 0$ and almost all $\underline{x}_n \in \partial\Gamma_n$, with respect to the measure $d\sigma_n$.

Remark. The continuity property stated in the above lemma is a consequence of the Liouville Equation, and it does not imply the stronger "continuity along trajectories", i.e. properties *(i)* and *(ii)* in the Remark (1) of Section 4, which are in general not valid unless we assume Eq. (4.3) for the initial measure.

Proof. We will deal first with correlation functions. For $n = N$ the claim is a trivial consequence of the Liouville equation (4.5), since the considered function is constant in time.

Suppose that the property holds for the function ρ_{n+1} for some $n \leq N-1$. Take $\varepsilon > 0$ small, and define $\Gamma_1^{(+\varepsilon)}(\underline{x}_n)$ as the one–particle configurations x_{n+1} compatible with $\underline{x}_n$ and such that the evolution $T_s^{(n+1)}$ does not lead to a collision of the $(n+1)-$th particle with the others in the time interval $s \in (0,\varepsilon]$. Then we have

$$\begin{aligned} &\Big| \int_{\Gamma_1(T^{(n)}_{t+\varepsilon+}(\underline{x}_n))} dx_{n+1}\rho_{n+1}\left(T^{(n)}_{t+\varepsilon+}(\underline{x}_n), x_{n+1}, t+\varepsilon\right) \qquad \text{(D.3)}\\ &\qquad - \int_{\Gamma_1(T^{(n)}_{t+}(\underline{x}_n))} dx_{n+1}\rho_{n+1}\left(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}, t\right) \Big| \\ &= \Big| \int_{\Gamma_1^{(+\varepsilon)}(T^{(n)}_{t+}(\underline{x}_n))} dx_{n+1}\rho_{n+1}\left(T^{(n+1)}_{\varepsilon+}(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}), t+\varepsilon\right) \\ &\qquad + O(\varepsilon) - \int_{\Gamma_1(T^{(n)}_{t+}(\underline{x}_n))} dx_{n+1}\rho_{n+1}\left(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}, t\right) \Big| \,. \end{aligned}$$

The term $O(\varepsilon)$ is the restriction of the integral in the first term of the first line to the points that, evolved backwards in time together with the configuration of particles $T^{(n)}_{t+\varepsilon+}(\underline{x}_n)$, display a collision with one of these particles in the time interval $(t, t+\varepsilon]$: explicitly it can be written, with the usual change of variables, as

$$\begin{aligned} &\sum_{j=1}^{n} \int_0^{\varepsilon} dt_1 \int_{\mathbb{R}^3} d\hat{p}_1 \int_{\Omega_{j+}^{(+\varepsilon)}(T^{(n)}_{t+t_1+}(\underline{x}_n), \hat{p}_1)} d\hat{\omega}_1 a^2 \hat{\omega}_1 \cdot (\hat{p}_1 - p_j(t+t_1)) \\ &\qquad \cdot \rho_{n+1}\left(T^{(n)}_{t+\varepsilon+}(\underline{x}_n), T^{(1)}_{-t_1+\varepsilon+}(q_j(t+t_1) + a\hat{\omega}_1, \hat{p}_1), t+\varepsilon\right) \,, \qquad \text{(D.4)} \end{aligned}$$

where here $p_j(t+t_1) = \left(T^{(n)}_{t+t_1+}(\underline{x}_n)\right)_{p_j}, q_j(t+t_1) = \left(T^{(n)}_{t+t_1+}(\underline{x}_n)\right)_{q_j}$, and $\Omega_{j+}^{(+\varepsilon)}(\cdots)$ denotes the subset of Ω_{j+} selecting particles that do not collide with the others when evolved forward in times of the interval $(t+t_1, t+\varepsilon]$. Clearly the term in (D.4) goes to zero as ε for $\varepsilon \longrightarrow 0$ in our assumptions.

A term similar to (D.4) is given by

$$\int_{\Gamma_1(T^{(n)}_{t+}(\underline{x}_n)) \setminus \Gamma_1^{(+\varepsilon)}(T^{(n)}_{t+}(\underline{x}_n))} dx_{n+1}\rho_{n+1}\left(T^{(n+1)}_{\varepsilon+}(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}), t+\varepsilon\right) = O(\varepsilon) \,. \qquad \text{(D.5)}$$

Hence (D.3) becomes

$$\begin{aligned} &\Big| \int_{\Gamma_1(T^{(n)}_{t+}(\underline{x}_n))} dx_{n+1}\Big[\rho_{n+1}\left(T^{(n+1)}_{\varepsilon+}(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}), t+\varepsilon\right) \qquad \text{(D.6)}\\ &-\rho_{n+1}\left(T^{(n)}_{t+}(\underline{x}_n), x_{n+1}, t\right)\Big]\Big| + O(\varepsilon) \,. \end{aligned}$$

Dominated convergence and the inductive assumption imply that this flows to zero with ε. A similar analysis can be performed for negative ε, therefore we have shown that, for all $\underline{x}_n \in \Gamma_n^{\dagger}$,

$$\lim_{\varepsilon \to 0^+} \rho_n(T^{(n)}_{t\pm\varepsilon}(\underline{x}_n), t \pm \varepsilon) = \rho_n(T^{(n)}_{t\pm}(\underline{x}_n), t) \qquad \text{(D.7)}$$

for any $t > 0$, which means continuity of the function in (D.1) for those t such that $T_t^{(n)}(\underline{x}_n) \notin \partial\Gamma_n$.

To deal with the collision configurations, notice that, for all $\underline{x}_n \in \Gamma_n^\dagger$,

$$\rho_n(T_{t+}^{(n)}(\underline{x}_n), t) = \rho_n(T_{t-}^{(n)}(\underline{x}_n), t) \tag{D.8}$$

for all $t > 0$, even if this is not true for the initial measure (this property must not be confused with the "continuity along trajectories", see Eq. (4.3)). In fact, for $n = N$ Eq. (D.8) is again a trivial consequence of the Liouville equation, while for $n < N$, it is easily proved by induction: assuming it for ρ_{n+1},

$$\begin{aligned}
\rho_n(T_{t+}^{(n)}(\underline{x}_n), t) &= \int_{\Gamma_1(T_{t+}^{(n)}(\underline{x}_n))} dx_{n+1}\rho_{n+1}(T_{t+}^{(n)}(\underline{x}_n), x_{n+1}, t) \\
&= \int_{\Gamma_1(T_{t-}^{(n)}(\underline{x}_n))} dx_{n+1}\rho_{n+1}(T_{t-}^{(n)}(\underline{x}_n), x_{n+1}, t) \\
&= \rho_n(T_{t-}^{(n)}(\underline{x}_n), t) \ ,
\end{aligned} \tag{D.9}$$

Equation (D.8), together with (D.7), prove the first assertion of the lemma for the correlation functions.

Coming now to the functions $V(\overline{\mathcal{D}})$ and remembering the explicit expression (3.10), we observe that $V(\overline{\mathcal{D}})(T_{t\pm\varepsilon\pm}^{(n)}(\underline{x}_n), t \pm \varepsilon) = \int_0^{t\pm\varepsilon} dt_1 \cdots$, where the dots indicate a function that depends only on the states of the evolution $\mathcal{E}_{\mathcal{D}}, \mathcal{D} = (T_{t\pm\varepsilon\pm}^{(n)}(\underline{x}_n), m, j_1, \cdots, j_m, t_1, \cdots, t_m, \hat{p}_1, \cdots, \hat{p}_m, \hat{w}_1, \cdots, \hat{w}_m)$, during the time interval $[0, t_1]$. Then for any $t_1 \in (0, t)$ this function is actually independent on ε: we can substitute $T_{t\pm\varepsilon\pm}^{(n)}(\underline{x}_n)$ in $\mathcal{D}$ with $T_{t\pm}^{(n)}(\underline{x}_n)$. Thus we obtain $V(\overline{\mathcal{D}})(T_{t\pm\varepsilon\pm}^{(n)}(\underline{x}_n), t \pm \varepsilon) = \int_0^t dt_1 \cdots + \int_t^{t\pm\varepsilon} dt_1 \cdots$, where the first term concides with $V(\overline{\mathcal{D}})(T_{t\pm}^{(n)}(\underline{x}_n), t)$, and the second term can be bounded, proceeding as after (3.10), with $O(\varepsilon)$. This shows that property (D.7) holds also for the function $V(\overline{\mathcal{D}})$, while property (D.8) is obvious for $V(\overline{\mathcal{D}})$, so that the claimed continuity property is proved for all $\underline{x}_n \in \Gamma_n^*$ and all $t > 0$.

Finally, to prove the statement over almost all $\partial\Gamma_n$, it suffices to apply the second part of Lemma A.0.1. □

Appendix E

Positivity of the activity

In this appendix we check that the constant introduced by (7.27) in the proof of Theorem 7.2.1 is well defined and positive. We put $x_j = (q_j, p_j)$. Using assumption (7.8) and the very definition of correlation functions, Eq. (7.3), we can easily rewrite the denominator in (7.27) as

$$\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_{(\Lambda\times\mathbb{R}^\nu)^k} dx_1 \cdots dx_k \prod_{j=1}^{k} \left(1 - e^{-\beta\varphi(q_j)}\right) \overline{\rho}_k(x_1, \cdots, x_k) \tag{E.1}$$
$$= \sum_{k=0}^{\infty} \sum_{p=0}^{k} \frac{(-1)^p}{p!(k-p)!} \int_{(\Lambda\times\mathbb{R}^\nu)^k} dx_1 \cdots dx_k \prod_{j=1}^{p} \left(1 - e^{-\beta\varphi(q_j)}\right) \mu_\Lambda^{(k)}(x_1, \cdots, x_k) \ ,$$

where the term $k = 0$ has to be interpreted as 1, and Λ is any open region containing the ball centered in 0 and with radius equal to the range of φ. Expanding the product, the integral in this expression is

$$\sum_{n=0}^{p} (-1)^n \int_{(\Lambda\times\mathbb{R}^\nu)^k} dx_1 \cdots dx_k \sum_{1\le j_1 < \cdots < j_n \le p} \left(\prod_{i=1}^{n} e^{-\beta\varphi(q_{j_i})} \right) \mu_\Lambda^{(k)}(x_1, \cdots, x_k)$$
$$= \sum_{n=0}^{p} (-1)^n \binom{p}{n} C_\Lambda^{(k,n)} \ , \tag{E.2}$$

where the equality holds by symmetry of $\mu_\Lambda^{(k)}$, with

$$C_\Lambda^{(k,n)} := \int_{(\Lambda\times\mathbb{R}^\nu)^k} dx_1 \cdots dx_k \left(\prod_{i=1}^{n} e^{-\beta\varphi(q_i)} \right) \mu_\Lambda^{(k)}(x_1, \cdots, x_k) \ . \tag{E.3}$$

Putting (E.2) into (E.1) and interchanging the sums, we have

$$\begin{aligned}
&\sum_{k=0}^{\infty}\frac{1}{k!}\sum_{n=0}^{k}\frac{(-1)^n}{n!}C_\Lambda^{(k,n)}\sum_{p=n}^{k}(-1)^p\frac{k!}{(k-p)!(p-n)!}\\
&=\sum_{k=0}^{\infty}\frac{1}{k!}\sum_{n=0}^{k}\frac{1}{n!}C_\Lambda^{(k,n)}\sum_{p=0}^{k-n}(-1)^p\frac{k!}{(k-n-p)!p!}\\
&=\sum_{k=0}^{\infty}\frac{1}{k!}\sum_{n=0}^{k}\frac{1}{n!}C_\Lambda^{(k,n)}k(k-1)\cdots(k-n+1)\delta_{n,k}\\
&=\sum_{k=0}^{\infty}\frac{1}{k!}C_\Lambda^{(k,k)}\ .
\end{aligned} \tag{E.4}$$

Since $\mu_\Lambda^{(k)} \geq 0$, this is a positive quantity. Condition (7.6) implies that it is different from zero.

Appendix F

Proof of (7.56)

Let us compute the right hand side of formula (7.56) for a sequence of smooth potentials $\varphi^{(\varepsilon)}$ approaching the hard core potential φ_d, as introduced in Chapter 8, see Eq. (8.8). We assume that the functions $\varphi^{(\varepsilon)}$ have support contained in the ball $B_d(0)$ centered in 0 and with radius $d > 0$.

After a change of variables the right hand side of (7.56) becomes (notice that we can always interchange the inner integrals)

$$\int_{\mathbb{R}^\nu} dy_1 \int_{-\infty}^0 d\bar{q}(1 - e^{-\beta\varphi^{(\varepsilon)}(\bar{q}-y_1)}) \int_{\mathbb{R}^\nu} dy_2 \frac{\partial(1 - e^{-\beta\varphi^{(\varepsilon)}(\bar{q}-y_1-y_2)})}{\partial\bar{q}} e^{-\beta\varphi^{(\varepsilon)}(y_2)} \ . \tag{F.1}$$

Consider the function on $\mathbb{R}^\nu$ defined by

$$\mathcal{B}^{(\varepsilon)}(x) = \int_{\mathbb{R}^\nu} dy(1 - e^{-\beta\varphi^{(\varepsilon)}(y-x)})e^{-\beta\varphi^{(\varepsilon)}(y)} \ : \tag{F.2}$$

this is smooth as the potential $\varphi^{(\varepsilon)}$ and

$$\mathcal{B}^{(\varepsilon)}(x) \underset{\varepsilon\to 0}{\longrightarrow} \mathcal{B}_d(x) \ , \tag{F.3}$$

where $\mathcal{B}_d(x)$ is the volume of the ball $B_d(x)$ centered in x minus its intersection with $B_d(0)$. The limit $\mathcal{B}_d(x)$ is continuous and differentiable in $x \neq 0$ for $d = 2, 3$ (and in $x \neq 0, \pm 2a$ for $d = 1$), with bounded derivative. We can write (F.1) as

$$\int_{\mathbb{R}^\nu} dy \int_{-\infty}^0 d\bar{q}(1 - e^{-\beta\varphi^{(\varepsilon)}(\bar{q}-y)}) \frac{\partial\mathcal{B}^{(\varepsilon)}(\bar{q}-y)}{\partial\bar{q}} \ . \tag{F.4}$$

Notice that by symmetry all the integrals are in fact over finite regions (the integral in dy can be restricted to $B_d(0)$, hence the integral in $d\bar{q}$ can be restricted to the interval $(-2d, 0)$), and that $\frac{\partial\mathcal{B}^{(\varepsilon)}(\bar{q}-y)}{\partial\bar{q}} \underset{\varepsilon\to 0}{\longrightarrow} \frac{\partial\mathcal{B}_d(\bar{q}-y)}{\partial\bar{q}}$ almost surely in $d\bar{q}$. By dominated convergence we can take the limit inside the integrals in (F.4), and we have

$$\int_{B_d(0)} \int_{-2d}^0 d\bar{q}\chi_<(\bar{q}-y) \frac{\partial\mathcal{B}(\bar{q}-y)}{\partial\bar{q}} \tag{F.5}$$

where $\chi_<(x)$ is the characteristic function of $|x| < d$. Performing the integral in $d\bar{q}$ we obtain the explicit result

$$\int_{B_d(0)} dy \mathcal{B}_d(y) - |B_d| B_d(d) \ , \tag{F.6}$$

where $|B_d|$ is the volume of the ball of radius d.

Now, suppose that formula (7.56) is *not* true, i.e. that the equality holds. Then

$$\begin{aligned}
&\int_{\mathbb{R}^\nu} dy_1 \int_{\mathbb{R}^\nu} dy_2 \int_{-\infty}^0 d\bar{q}(1 - e^{-\beta\varphi^{(\varepsilon)}(\bar{q}-y_1)}) \frac{\partial(1 - e^{-\beta\varphi^{(\varepsilon)}(\bar{q}-y_2)})}{\partial\bar{q}} e^{-\beta\varphi^{(\varepsilon)}(y_1-y_2)} \\
&= \frac{1}{2}\int_{\mathbb{R}^{2\nu}} dy_1 dy_2 (1 - e^{-\beta\varphi^{(\varepsilon)}(y_1)})(1 - e^{-\beta\varphi^{(\varepsilon)}(y_2)}) e^{-\beta\varphi^{(\varepsilon)}(y_1-y_2)} \\
&= \frac{1}{2}\int_{\mathbb{R}^{2\nu}} dy_1 dy_2 (1 - e^{-\beta\varphi^{(\varepsilon)}(y_1)})(1 - e^{-\beta\varphi^{(\varepsilon)}(y_1-y_2)}) e^{-\beta\varphi^{(\varepsilon)}(y_2)} \\
&= \frac{1}{2}\int_{\mathbb{R}^\nu} dy (1 - e^{-\beta\varphi^{(\varepsilon)}(y)}) \mathcal{B}_d^{(\varepsilon)}(y) \ ,
\end{aligned} \tag{F.7}$$

where in the first equality we integrated by parts using symmetry for exchange of y_1, y_2 (and the fact that (7.56) is not true) and in the second equality we performed again a change of variables. The result in the limit $\varepsilon \longrightarrow 0$ is

$$\frac{1}{2}\int_{B_d(0)} dy \mathcal{B}_d(y) \ , \tag{F.8}$$

which is different from (F.6) (easy calculation shows that for $\nu = 1, 2, 3$ respectively it is $|B_d|\mathcal{B}_d(d) = 2d^2, \pi d^4(\frac{\pi}{3} + \frac{\sqrt{3}}{2}), \frac{11}{9}\pi^2 d^6$, while $\frac{1}{2}\int_{B_d(0)} dy \mathcal{B}_d(y) = \frac{d^2}{2}, \frac{3\sqrt{3}}{8}\pi d^4, \frac{17}{36}\pi^2 d^6$). Thus we got a contradiction. $\square$

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