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► **To cite this version:**

Mario Pulvirenti, Sergio Simonella, Anton Trushechkin. Microscopic solutions of the Boltzmann-Enskog equation in the series representation. *Kinetic and Related Models*, 2018, 11 (4), pp.911-931. hal-01956021

HAL Id: hal-01956021

<https://hal.science/hal-01956021>

Submitted on 14 Dec 2018

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Microscopic solutions of the Boltzmann–Enskog equation in the series representation

Mario Pulvirenti, Sergio Simonella and Anton Trushechkin

MARIO PULVIRENTI

International Research Center M&MOCS, Università dell’Aquila
Palazzo Caetani, Cisterna di Latina, (LT) 04012, Italy

SERGIO SIMONELLA

CNRS and UMPA (UMR CNRS 5669), École Normale Supérieure de Lyon
46 allée d’Italie, 69364 Lyon Cedex 07, France

ANTON TRUSHECHKIN

Steklov Mathematical Institute of Russian Academy of Sciences
Gubkina Street 8, Moscow 119991, Russia
National Research Nuclear University MEPhI
Kashirskoe Highway 31, Moscow 115409, Russia
National University of Science and Technology MISIS
Leninsky Avenue 2, Moscow 119049, Russia

Abstract

The Boltzmann–Enskog equation for a hard sphere gas is known to have so called microscopic solutions, i.e., solutions of the form of time-evolving empirical measures of a finite number of hard spheres. However, the precise mathematical meaning of these solutions should be discussed, since the formal substitution of empirical measures into the equation is not well-defined. Here we give a rigorous mathematical meaning to the microscopic solutions to the Boltzmann–Enskog equation by means of a suitable series representation.

1 Introduction

The present paper is devoted to the Boltzmann–Enskog equation, which describes the kinetics of a hard sphere gas:

$$\begin{aligned} (\partial_t + v \cdot \nabla_x) f(x, v, t) &= \lambda \int_{\mathbb{R}^3 \times S_+^2} dv_1 d\omega (v - v_1) \cdot \omega \\ &\times \left\{ f(x - a\omega, v_1', t) f(x, v', t) - f(x + a\omega, v_1, t) f(x, v, t) \right\}, \end{aligned} \quad (1)$$

where the unknown $f = f(x, v, t) \geq 0$ denotes the density function of the system, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$ and $t \in \mathbb{R}$ denote position, velocity and time respectively. Moreover $a > 0$ is the diameter of a hard sphere. If the function is normalized, i.e., $\int_{\mathbb{R}^6} f(x, v, t) dx dv = 1$, then f can be understood as a probability density of an arbitrary single hard sphere. Further, $S_+^2 = \{\omega \in S^2 \mid (v - v_1) \cdot \omega \geq 0\}$, S^2 is the unit sphere in \mathbb{R}^3 (with the surface measure $d\omega$), (v, v_1) is a pair of velocities in incoming

collision configuration and (v', v'_1) is the corresponding pair of outgoing velocities defined by the elastic reflection rules (with ω being the unit vector directed from the center of the first sphere to the center of the second one)

$$\begin{cases} v' = v - \omega[\omega \cdot (v - v_1)] \\ v'_1 = v_1 + \omega[\omega \cdot (v - v_1)]. \end{cases} \quad (2)$$

Finally, $\lambda > 0$ is a parameter modulating the collision rate. The integral in (1) is referred to as the collision integral.

This equation differs from the Boltzmann kinetic equation for hard spheres by the terms $\pm a\omega$ in the arguments of f in the collision integral. Namely the Boltzmann equation assumes the size of spheres to be negligibly small (in comparison to the scale of spatial variation of f), while the Boltzmann–Enskog equation takes the size of spheres into account. Formally, the Boltzmann equation for hard spheres is obtained from the Boltzmann–Enskog equation in the limit $a \rightarrow 0$. The convergence of solutions of the Boltzmann–Enskog equation to solutions of the Boltzmann equation is proved in [2, 3, 4]. Thus Eq. (1) is often regarded as a correction to the Boltzmann equation which is both a simpler mathematical model and a kinetic description of a “dense gas”.

An important problem in the theory of the Boltzmann equation is its derivation from the microscopic dynamics (Hamiltonian particle system), see [8, 22, 12, 16] and, for more recent research, [7, 15, 14, 20, 18, 13]. Up to now, the Boltzmann equation for hard spheres and other short-range potentials has been rigorously derived for short times only. In contrast to the Boltzmann equation, it is not clear whether an Enskog type equation can be rigorously derived from deterministic dynamics.

It is interesting that, in case of hard spheres, Bogolyubov’s microscopic derivation in [8] leads not to the Boltzmann equation but to the Boltzmann–Enskog equation (1). However, the latter equation does not provide a better approximation to the hard sphere dynamics, but just a natural intermediate description [20].

Moreover, the Boltzmann–Enskog equation has an interesting property, which relates it to the microscopic dynamics in a different way. Namely, Bogolyubov discovered [9] (see also [10]) that, for any finite N , the Boltzmann–Enskog equation with $\lambda = Na^2$ has solutions of the form of time-evolving empirical measures of N hard spheres:

$$\mu_t(dz) = \frac{1}{N} \sum_{i=1}^N \delta(z - z_i(t)) dz. \quad (3)$$

Here $z = (x, v) \in \mathbb{R}^6$ is a point in the phase space and $z_i(t) = (x_i(t), v_i(t))$ is the phase point of the i -th hard sphere determined by free motion between collisions plus elastic pairwise reflections at distance a . Setting $\mathbf{z}(t) = (z_i(t))_{i=1}^N = \mathbb{T}_N(t)\mathbf{z}^0$, and $\mathbf{z}^0 = (z_i^0)_{i=1}^N$ the time evolved and initial configuration respectively, the flow $\mathbf{z}^0 \rightarrow \mathbf{z}(t)$ is defined for almost all \mathbf{z}^0 with respect to the Lebesgue measure. In fact configurations leading to collisions of more than two hard spheres simultaneously, to grazing collisions or to infinite collisions in a finite time have zero measure [1, 11, 12].

Solutions of type (3) are referred to as microscopic solutions. It may be surprising that the Boltzmann–Enskog equation “contains” the N -particle dynamics in itself, while the kinetic equation is valid in the limit of large N only.

Such solutions are even more surprising if we recall that the Boltzmann–Enskog equation describes the irreversible dynamics of the gas. Namely, consider the functional

$$H(f) = \int_{\mathbb{R}^6} f \ln f \, dx dv + \frac{\lambda}{2} \int_{\mathbb{R}^3} dx \int_{B(x,a)} \rho(x) \rho(y) \, dy, \quad (4)$$

where $B(x, a)$ is the ball around x and radius a , and $\rho(x) = \int_{\mathbb{R}^3} f(x, v) \, dv$ is the spatial density. This functional does not increase if f is a solution of the Boltzmann–Enskog equation [3]. In contrast, microscopic solutions are reversible in time (i.e., a transformation $t \rightarrow -t$ and $v \rightarrow -v$ maps a measure of type (3) to another measure of this type, which is also a solution of (1)). Of course, functional (4) is not defined on solutions of type (3), hence, formally, there is no contradiction. However, this shows that the reversibility or irreversibility of the Boltzmann–Enskog equation depends on the considered class of solutions: we have irreversible behaviour if we consider regular solutions, and reversible behaviour in the case of suitable singular measures (3).

A difficulty with the microscopic solutions (3) is that their formal substitution into (1) yields products of delta functions and, hence, it is ill-defined. A rigorous sense to these solutions was given in [25] by means of regularizations for delta functions and the collision integral (see also [23, 26] for other variants). On the other hand it was proven in [19] that the empirical distributions (3) (more precisely the family of the empirical marginals) solve the BBGKY hierarchy for hard spheres. Actually, Bogolyubov’s remark in [9] was that the Boltzmann–Enskog equation coincides formally with the first equation of the BBGKY hierarchy for hard spheres.

As discussed in [19], the approach therein developed, based on the standard notion of Duhamel series solution, has no simple adaptation to (1). In the present paper, we introduce a modified notion of series solution for which (3) does solve the Boltzmann–Enskog equation. Such a notion is based on tree expansions with partially ordered trees, in contrast with the standard expansion on totally ordered trees. This, together with a regularization based on separation of collision times, allows to formulate our main result (Theorem 4.1 in Section 4 below).

The paper is organized as follows. In Section 2 we introduce the trees and partially ordered trees together with the standard series solution. In Section 3 the concept of series solution for measures of type (3) is precisely formulated. We establish also a semigroup property which will be crucial, in Section 4, for the proof of Theorem 4.1. In the latter section we finally compare the strategy of [19] with the one of the present paper.

2 Series solution and tree expansion

2.1 Series expansion and trees

We will use the following notations: $\mathbf{z}_j = (z_1, \dots, z_j)$, $z_i = (x_i, v_i)$,

$$f^{\otimes j}(\mathbf{z}_j, t) = f(z_1, t) \cdots f(z_j, t).$$

Also, for shortness, we will write $f(t)$ and $f^{\otimes j}(t)$ for $f(z_1, t)$ and $f^{\otimes j}(\mathbf{z}_j, t)$ respectively. Let us introduce the operators $\mathcal{S}_i(t)$ and $\mathcal{C}_{i,j+1}^\pm$:

$$(\mathcal{S}_i(t) f^{\otimes j})(\mathbf{z}_j, t) = f(z_1, t) \cdots f(z_{i-1}, t) f(x_i - v_i t, v_i, t) f(z_{i+1}, t) \cdots f(z_j, t),$$

$$\begin{aligned} \left(\mathcal{C}_{i,j+1}^+ f^{\otimes(j+1)} \right) (\mathbf{z}_j, t) &= \int_{\mathbb{R}^3 \times S_+^2} dv_{j+1} d\omega_{j+1} (v_i - v_{j+1}) \cdot \omega_{j+1} \\ &\times f(z_1, t) \cdots f(z_{i-1}, t) f(x_i, v'_i, t) f(z_{i+1}, t) \cdots f(z_j, t) f(x_i - a\omega_{j+1}, v'_{j+1}, t), \end{aligned}$$

$$\begin{aligned} \left(\mathcal{C}_{i,j+1}^- f^{\otimes(j+1)} \right) (\mathbf{z}_j, t) &= \int_{\mathbb{R}^3 \times S_+^2} dv_{j+1} d\omega_{j+1} (v_i - v_{j+1}) \cdot \omega_{j+1} \\ &\times f(z_1, t) \cdots f(z_{i-1}, t) f(x_i, v_i) f(z_{i+1}, t) \cdots f(z_j, t) f(x_i + a\omega_{j+1}, v_{j+1}, t), \\ \mathcal{C}_{i,j+1} &= \mathcal{C}_{i,j+1}^+ - \mathcal{C}_{i,j+1}^-. \end{aligned}$$

We remind that $S_+^2 = \{\omega \in S^2 \mid (v - v_1) \cdot \omega \geq 0\}$ and S^2 is the unit sphere in \mathbb{R}^3 . Then, the Boltzmann–Enskog equation (1) can be rewritten as

$$(\partial_t + v_1 \cdot \nabla_{x_1}) f(t) = \lambda \mathcal{C}_{1,2} f^{\otimes 2}(t),$$

or, in the integrated form, as

$$f(t) = \mathcal{S}_1(t) f_0 + \lambda \int_0^t ds \mathcal{S}_1(t-s) \mathcal{C}_{1,2} f(s) f(s), \quad (5)$$

where $f_0 \equiv f_0(z_1)$.

If we iterate equation (5) (i.e., iteratively substitute (5) into the right-hand side of itself), we obtain a series solution in the form

$$\begin{aligned} f_j(t) &= \mathcal{S}_{1\dots j} f_{0,j} + \sum_{n=1}^{\infty} \lambda^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \\ &\mathcal{S}_{1\dots j}(t-t_1) \mathcal{C}_{j+1} \mathcal{S}_{1\dots j+1}(t_1-t_2) \dots \mathcal{C}_{j+n} \mathcal{S}_{1\dots j+n}(t_n) f_{0,j+n}, \quad (6) \end{aligned}$$

where $f_j(t) = f^{\otimes j}(t)$, $f_{0,j+n} = f_0^{\otimes(j+n)}$,

$$\mathcal{C}_j = \sum_{l=1}^{j-1} \mathcal{C}_{l,j}, \quad (7)$$

and $\mathcal{S}_{1\dots j}(s) = \mathcal{S}_1(s) \dots \mathcal{S}_j(s)$. The substitution of (7) into (6) yields

$$\begin{aligned} f_j(t) &= \mathcal{S}_{1\dots j} f_{0,j} + \sum_{n=1}^{\infty} \lambda^n \sum_{\mathbf{r}_n}^* \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \\ &\mathcal{S}_{1\dots j}(t-t_1) \mathcal{C}_{r_1,j+1} \mathcal{S}_{1\dots j+1}(t_1-t_2) \dots \mathcal{C}_{r_n,j+n} \mathcal{S}_{1\dots j+n}(t_n) f_{0,j+n}, \quad (8) \end{aligned}$$

where

$$\sum_{\mathbf{r}_n}^* = \sum_{r_1=1}^j \sum_{r_2=1}^{j+1} \cdots \sum_{r_n=1}^{j+n-1}.$$

Expansion (8) leads to a natural tree representation, where r_i is a ‘parent’ of the particle $j+i$. (Again, if we are interested only on the single-particle distribution function, we should set $j=1$. Here we are introducing the ‘hierarchy’ of equations for the functions f_j , which will be useful in the sequel.)

The collection of integers

$$\mathbf{r}_n = \{r_1, \dots, r_n\}$$

is called ‘tree’. The name is justified by the fact that a tree is conveniently represented graphically. For instance the tree $\mathbf{r}_5 = \{1, 1, 2, 3, 2\}$ for $j=1$ is given by Fig. 1 where the i -th branch is generated by particle r_i ; see also Figure 2.

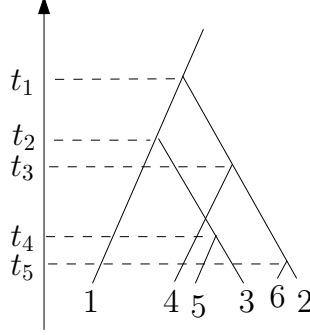


Figure 1: : $\mathbf{r}_5 = \{1, 1, 2, 3, 2\}$.

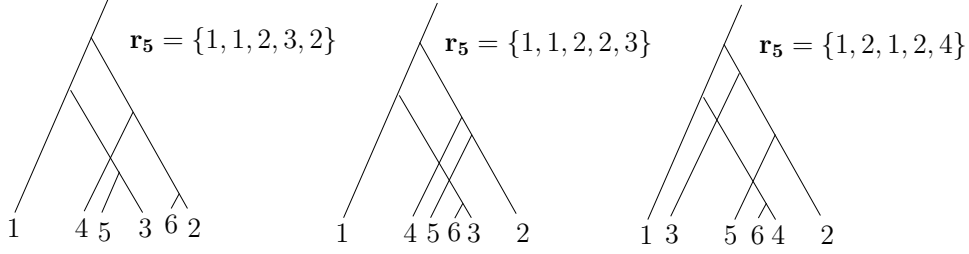


Figure 2:

Remark 1 For the tree representation we refer to [22] (“Collision Histories”). Later on this notion has been used frequently by several authors [17, 14, 18, 19, 20, 21, 5, 6].

The series expansion (8) can be further specified by splitting any operator \mathcal{C}_j into its positive and negative part. The result is:

$$f_j(t) = \mathcal{S}_{1\dots j} f_{0,j} + \sum_{n=1}^{\infty} \lambda^n \sum_{\mathbf{r}_n}^* \sum_{\boldsymbol{\sigma}_n} \prod_{i=1}^n \sigma_i \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \\ \mathcal{S}_{1\dots j}(t-t_1) \mathcal{C}_{r_1, j+1}^{\sigma_1} \mathcal{S}_{1\dots j+1}(t_1-t_2) \dots \mathcal{C}_{r_n, j+n}^{\sigma_n} \mathcal{S}_{1\dots j+n}(t_n) f_{0, j+n}, \quad (9)$$

where $\boldsymbol{\sigma}_n = \{\sigma_1, \dots, \sigma_n\}$ and $\sigma_i = \pm$.

2.2 Backward and forward Boltzmann–Enskog flows

The operators $\mathcal{C}_{r_i, j+i}^{\sigma_i}$ are integrals over $d\omega_i$ and dv_{j+i} which, together with t_i , will be called the ‘node variables’ (see Fig. 1).

Given n , \mathbf{r}_n , $\boldsymbol{\sigma}_n$ and values of the node variables, we now define the so called *Boltzmann–Enskog backward flow* for the configuration of particles $\zeta(s)$, $s \in [0, t]$,

$$\zeta(s) = (\zeta_i(s))_{i \in \mathcal{H}(s)}, \quad \mathcal{H}(s) = \{1\} \cup \{i \geq 2 \mid t_{i-1} \geq s\}, \quad (10)$$

with $\zeta_i(s) = (\xi_i(s), \eta_i(s))$, respectively position and velocity of particle i . Let us define the flow. Note that the number of particles is increasing backward in time.

We are considering the case $j = 1$ for simplicity.

Firstly,

$$\zeta(t) = \zeta_1(t) = (x_1, v_1) \quad (11)$$

(recall that (x_1, v_1) are the arguments of the function f_1 in (9)). At the instant t , only the first particle is under consideration. It moves freely, back in time, up to the instant of the first creation t_1 , i.e.

$$\zeta(t_1 + 0) = \zeta_1(t_1 + 0) = (x_1 - v_1 t_1, v_1).$$

The time instant t_1 corresponds to a contact with the particle 2 with the configuration $(x_1 - \sigma_1 a \omega_1, v_1)$ (“contact” means that the distance between the centres of the hard spheres is exactly a). We add the configuration of this particle to ζ . If $\sigma_1 = -$, then the configuration of the particles is precollisional and both particles continue to move freely (backward in time) with their velocities (v_1, v_2) , so that

$$\zeta(t_1 - 0) = (\zeta_1(t_1 - 0), \zeta_2(t_1 - 0)) = ((x_1 - v_1 t_1, v_1), (x_1 - v_1 t_1 + a \omega_1, v_2)).$$

If $\sigma_1 = +$, then the configuration of the particles is postcollisional, and the particles continue to move freely (backward in time) with the precollisional velocities (v'_1, v'_2) :

$$\zeta(t_1 - 0) = (\zeta_1(t_1 - 0), \zeta_2(t_1 - 0)) = ((x_1 - v_1 t_1, v'_1), (x_1 - v_1 t_1 - a \omega_1, v'_2)).$$

Both particles continue to move freely (backward in time) up to their next collision, and so on. Since r_i is the “parent particle” of the particle i , $i = 2, \dots, n + 1$, the general formula reads

$$\zeta_i(t_{i-1} - 0) = \begin{cases} (\xi_{r_i}(t_{i-1}) + a \omega_{i-1}, v_i), & \sigma_{i-1} = -, \\ (\xi_{r_i}(t_{i-1}) - a \omega_{i-1}, v'_i), & \sigma_{i-1} = +, \end{cases} \quad (12)$$

for $i = 2, \dots, n + 1$.

The above prescription defines the backward Boltzmann–Enskog flow.

Thus, given $t > 0$, we have a $(\mathbf{r}_n, \boldsymbol{\sigma}_n)$ -dependent map

$$(x_1, v_1, \mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n) \longmapsto \zeta(0), \quad (13)$$

where $\mathbf{t}_n = (t_1, \dots, t_n)$, $\boldsymbol{\omega}_n = (\omega_1, \dots, \omega_n)$, $\mathbf{v}_n = (v_2, \dots, v_{n+1})$. This map is important since it appears in formula (9), by writing explicitly the transport and collision operators.

The transformation (13) is a Borel map and we will denote its image as $\tilde{A}_{\mathbf{r}_n \boldsymbol{\sigma}_n}(t)$. Obviously, the image for $n = 0$ is \mathbb{R}^6 . The Jacobian determinant of the transformation is in modulus $a^{2n} \prod_{i=1}^n |\omega_i \cdot (v_{i+1} - \eta_{r_i}(t_i + 0))|$, so that the map induces the equivalence of measures

$$dx_1 dv_1 d\Lambda a^{2n} \prod_{i=1}^n |\omega_i \cdot (v_{i+1} - \eta_{r_i}(t_i + 0))| = d\zeta(0),$$

where

$$d\Lambda(\mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n) = \chi_{\mathbf{r}_n}(\mathbf{t}_n) dt_1 \dots dt_n d\omega_1 \dots d\omega_n dv_2 \dots dv_{n+1},$$

$$\chi_{\mathbf{r}_n}(\mathbf{t}_n) = \begin{cases} 1, & 0 < t_{i+1} < t_i \quad i = 0, \dots, n, \quad t_0 = t, t_{n+1} = 0 \\ 0, & \text{otherwise.} \end{cases}$$

We will use also the inverse of map (13). To construct it, we introduce the *Boltzmann–Enskog forward flow*, dependent on $(\mathbf{k}_n, \boldsymbol{\sigma}_n)$:

$$\zeta(0) \longmapsto (\zeta^F(s))_{s \in [0,t]} = (\zeta^F(s, \zeta(0), \mathbf{r}_n, \boldsymbol{\sigma}_n))_{s \in [0,t]}, \quad (14)$$

where $\zeta(0) \in \tilde{A}_{\mathbf{r}_n \boldsymbol{\sigma}_n}(t)$. A tree or, algebraically, the n -tuple \mathbf{r}_n prescribes the sequences of creations (i.e., collisions) of the n particles.

The Boltzmann–Enskog forward flow is defined as follows. A particle i moves freely up to a contact with some other particle j . If the particle j is not the next collision partner of the particle i or the particle i is not the next collision partner of the particle k , then they ignore each other, i.e., they go through each other reaching a mutual distance $\leq a$. Otherwise, if the two particles are the next collision partners as specified by \mathbf{r}_n , then the particle with the larger number disappears from ζ^F . For definiteness, let $i > k$, hence $k = r_i$. If $\sigma_{i-1} = -$, then the particle k does not change its velocity. If $\sigma_{i-1} = +$, then the particle k changes its velocity according to law (2) (with v and v_1 substituted by the precollisional velocities of the particles k and i respectively, and ω being the unit vector directed from the center of the hard sphere i to the center of the hard sphere k). If, according to the tree, the particles i and k are the next collision partners, then the existence of a moment of their contact is guaranteed by the condition $\zeta(0) \in \tilde{A}_{\mathbf{r}_n \boldsymbol{\sigma}_n}(t)$.

By construction, if we apply the backward flow (13) to $(x_1, v_1, \mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n)$ with $s = 0$ to obtain $\zeta(0)$ and then apply the forward flow to $\zeta(0)$, we will obtain $\zeta^F(t) = \zeta_1^F(t) = (x_1, v_1)$.

Remark 2 *It may be worth to underline that forward and backward flows are not directly connected with the real dynamics of a hard-sphere system. In these flows particles can overlap and the tree \mathbf{r}_n specifies which pair of particles must collide once at contact and which particles overlap freely. This formalism is just a way to represent the solution of a partial differential equation. A connection with the hard-sphere motion will be discussed later on.*

2.3 Partially ordered trees

Preliminary to the construction of measure valued solutions discussed in the next section, we introduce here a rearrangement of the previous series expansion, based on a different notion of tree which will be called ‘partially ordered tree’ in contrast with the fully ordered tree -or simply ‘tree’- defined above. Here we disregard the mutual ordering of collision times, except for those particles having the same parent. Equivalently, we ignore the time ordering of the birthdays of descendants of different parents.

For instance consider the tree $\mathbf{r}_5 = \{1, 1, 2, 3, 2\}$ in Fig. 1, and the other two trees in Fig. 2, in which the time ordering $t_5 < t_4$ and $t_3 < t_2$ is ignored. All these trees are equivalent to the first one as unlabelled graphs. We call then ‘partially ordered tree’ a tree in which only the ordering of branches generated by a given one is fixed. In Fig. 3 a partially ordered tree is the collection of a fully ordered trees with different ordering of the times t_2, t_3 and t_4, t_5 and so on.

Each partially ordered tree is fully specified by the sequence of integers

$$\mathbf{k}_n = \{k_1, \dots, k_n\}$$

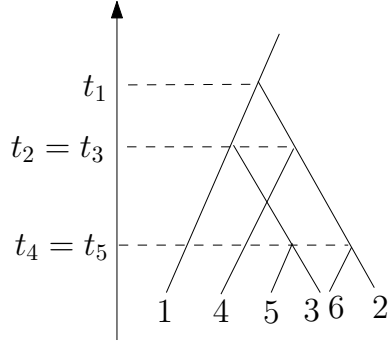


Figure 3:

where k_i is the number of collisions of the particle i on the way to its final point (after its creation). In particular, k_1 is the number of particles generated by the first particle. The name assigned to each particle is specified as follows.

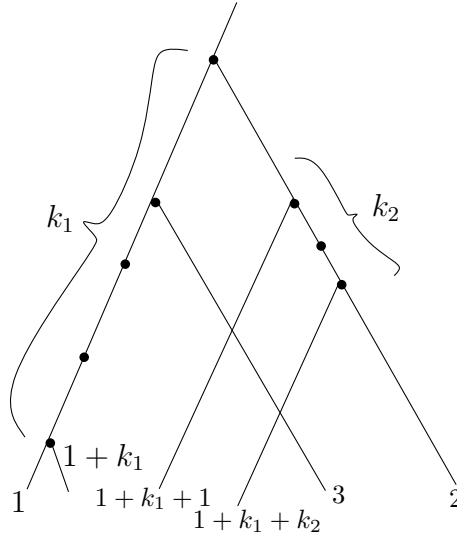


Figure 4:

Defining

$$K_i = \begin{cases} 1, & i = 1, \\ 1 + \sum_{l=1}^{i-1} k_l, & i > 1; \end{cases}$$

we fix the following ordering: particles created by particle i obtain the numbers $K_i + 1, \dots, K_i + k_i$. We also set $k_{n+1} := 0$, since the particle with the last number does not suffer collisions.

We denote the set of partially ordered trees by $\mathcal{K}_n = \{\mathbf{k}_n = (k_1, \dots, k_n)\} \subset$

$\{0, \dots, n\}^n$. We will use that it is given by n -tuples of integers such that

$$\sum_{i=1}^n k_i = n. \quad (15)$$

The variables k_i are related by the fact that the tree \mathbf{k}_n must be realizable as graph. For instance the sequence $(1, 0, 2, 1)$ with $n = 4$ is not admissible, because it contains descendants without parents. First, we require $k_1 \geq 1$ always. Then if $k_i > 0$, particle i must be already created in the procedure described above.

Note that we can represent the solution of the Boltzmann–Enskog equation in terms of partially ordered trees as

$$f(t) = \sum_{n=0}^{\infty} \lambda^n f^{(n)}(t), \quad (16)$$

$$f^{(0)}(t) = \mathcal{S}_1(t) f_0, \quad (17a)$$

$$f^{(n)}(t) = \sum_{\mathbf{k}_n \in \mathcal{K}_n} \mathcal{Q}_{\mathbf{k}_n}(1; t) f_0^{\otimes(n+1)}, \quad n \geq 1, \quad (17b)$$

where the operators \mathcal{Q} are given by the following recursive formula:

$$\begin{aligned} \mathcal{Q}_{\mathbf{k}_n}(i; s) = & \\ & \left[\prod_{j=0}^{k_i-1} \int_0^{T_{ij}} dt_{K_i+j} \mathcal{S}_i(T_{ij} - t_{K_i+j}) \mathcal{C}_{i, K_i+j+1} \mathcal{Q}_{\mathbf{k}_n}(K_i + j + 1; t_{K_i+j}) \right] \\ & \times \mathcal{S}_i(t_{K_i+k_i-1}) \end{aligned} \quad (18)$$

if $k_i \geq 1$ and $\mathcal{Q}_{\mathbf{k}_n}(i; s) = \mathcal{S}_i(s)$ if $k_i = 0$. Here

$$T_{ij} = \begin{cases} s, & j = 0, \\ t_{K_i+j-1}, & j > 0. \end{cases}$$

Then

$$\begin{aligned} \mathcal{Q}_{\mathbf{k}_n}(1; t) = & \int_0^t \mathcal{S}_1(t - t_1) \mathcal{C}_{1,2} \mathcal{Q}_{\mathbf{k}_n}(2; t_1) \int_0^{t_1} \mathcal{S}_1(t_1 - t_2) \mathcal{C}_{1,3} \mathcal{Q}_{\mathbf{k}_n}(3; t_2) \times \dots \\ & \times \int_0^{t_{k_1-1}} \mathcal{S}_1(t_{k_1-1} - t_{k_1}) \mathcal{C}_{1, k_1} \mathcal{Q}_{\mathbf{k}_n}(k_1; t_{k_1-1}) \mathcal{S}_1(t_{k_1}). \end{aligned}$$

For each $\mathcal{Q}_{\mathbf{k}_n}(\ell; t_{\ell-1})$ we repeat the procedure to arrive to Eq. (16).

Observe that the notions of backward and forward Boltzmann–Enskog flow, introduced in the previous section, can be extended easily to the present context. We define as before the $(\mathbf{k}_n, \boldsymbol{\sigma}_n)$ -dependent map

$$(x_1, v_1, \mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n) \mapsto \boldsymbol{\zeta}(0), \quad (19)$$

the only difference being that the times $\mathbf{t}_n = (t_1, \dots, t_n)$ are only partially ordered. Moreover we denote by $A_{\mathbf{k}_n \boldsymbol{\sigma}_n}(t)$ the image of this Borel map.

Notice that two fully ordered trees yield the same partially ordered tree if they are equivalent as topological (unlabelled) graphs. Therefore \mathbf{k}_n can be thought as an equivalence class of fully ordered trees and we write $\mathbf{r}_n \in \mathbf{k}_n$ if \mathbf{r}_n belongs to the equivalence class specified by \mathbf{k}_n . We have

$$\bigcup_{\mathbf{r}_n \in \mathbf{k}_n} \tilde{A}_{\mathbf{r}_n \sigma_n} = A_{\mathbf{k}_n \sigma_n}.$$

Moreover

$$\sum_{\mathbf{r}_n}^* = \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\mathbf{r}_n \in \mathbf{k}_n}.$$

The introduction of the backward Boltzmann–Enskog flow allows to write the series solution in a more explicit way, namely

$$\begin{aligned} f(x_1, v_1, t) &= \sum_{n=0}^{\infty} \lambda^n \sum_{\mathbf{k}_n} \sum_{\sigma_n \in \{\pm\}^n} \int d\Lambda \prod_{i=1}^n \sigma_i [\omega_i \cdot (v_{i+1} - \eta_{r_i}(t_i + 0))] f_0^{\otimes(n+1)}(\zeta(0)), \quad (20) \end{aligned}$$

where r_i is the parent of particle i in the partially ordered tree, $\zeta(0) = \zeta(0, \mathbf{k}_n, \sigma_n)$,

$$d\Lambda(\mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n) = \chi_{\mathbf{k}_n}(\mathbf{t}_n) dt_1 \dots dt_n d\omega_1 \dots d\omega_n dv_2 \dots dv_{n+1},$$

$\chi_{\mathbf{k}_n}(\mathbf{t}_n)$ is the indicator function of the partial order dictated by the tree \mathbf{k}_n and $\zeta(s, \mathbf{k}_n, \sigma_n)$, $s \in (0, t)$ is the backward flow. By using the change of variables induced by the map (19), we arrive to

$$\begin{aligned} &\int dz_1 f(x_1, v_1, t) \phi(z_1) \\ &= \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \int_{A_{\mathbf{k}_n \sigma_n}(t)} dz_{n+1} f_0^{\otimes(n+1)}(\mathbf{z}_{n+1}) \phi(\zeta_1(t)), \quad (21) \end{aligned}$$

for any bounded continuous function $\phi : \mathbb{R}^6 \rightarrow \mathbb{R}$.

A fundamental property of the series expansion is the semigroup property. Denote $\mathcal{T}(t)$ the evolution operator sending f_0 to $f(t)$, as given by the above formulas. Then $f(t) = \mathcal{T}(t)f_0$. If $\tau_1, \tau_2 \geq 0$, then by algebraic manipulations it follows that

$$\mathcal{T}(\tau_1 + \tau_2) = \mathcal{T}(\tau_2)\mathcal{T}(\tau_1). \quad (22)$$

In Section 3, more attention will be paid to the proof of the semigroup property for measure valued solutions, which will be needed to construct the microscopic solutions of the Boltzmann–Enskog equation.

2.4 Convergence

The first relevant property of the expansion in terms of partially ordered trees is that their number is much smaller than the number of fully ordered trees. Indeed, while

$$\sum_{\mathbf{r}_n} 1 = n!,$$

$$\sum_{\mathbf{k}_n \in \mathcal{K}_n} 1 \leq \sum_{\substack{k_1, \dots, k_n \geq 0, \\ k_1 + \dots + k_n = n}} 1 = \sum_{\substack{k_1, \dots, k_n \geq 0, \\ k_1 + \dots + k_n = n}} 2^n \prod_{i=1}^n 2^{-k_i} < 4^n .$$

This allows to prove

Proposition 1 *If $\lambda < a^2/8\|f_0\|$ (where $\|\cdot\|$ is the L^1 -norm), the series (21) is convergent (in $L^1(\mathbb{R}^6)$) for all $t > 0$.*

Proof. We have

$$\|f(t)\| \leq \|f_0\| + \sum_{n=1}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \int_{A_{\mathbf{k}_n \sigma_n}(t)} f_0^{\otimes(n+1)}(\zeta_{n+1}) d\zeta_{n+1} .$$

The generic term is smaller than

$$\begin{aligned} & \left(\frac{\lambda}{a^2}\right)^n \|f_0\|^{n+1} \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} 1 = \left(\frac{2\lambda}{a^2}\right)^n \|f_0\|^{n+1} \sum_{\mathbf{k}_n \in \mathcal{K}_n} 1 \\ & \leq \left(\frac{2\lambda}{a^2}\right)^n \|f_0\|^{n+1} \sum_{\substack{k_1, \dots, k_n \geq 0, \\ k_1 + \dots + k_n = n}} 1 < \left(\frac{8\lambda}{a^2}\right)^n \|f_0\|^{n+1} . \end{aligned}$$

We see that the series geometrically converges whenever $\lambda < a^2/8\|f_0\|$.

This slightly improves the result of [17] due to another algebraic way of description of the same graphical tree structure: we specify a tree just by an n -tuple \mathbf{k}_n .

Moreover it may be interesting to observe that one can prove the convergence for any λ , but small t . However, this is not a real restriction, since the free energy functional (4) provides a uniform (in time) estimate of absolute continuity of the distribution function which allows to iterate the procedure to reach arbitrary times, see [17].

3 Measure valued solutions

To prove the existence of microscopic solutions to the Enskog equation, we need to extend the series solution discussed so far to the case of initial singular measures. Proceeding formally we write, for any bounded continuous $\varphi(x_1, v_1)$ on \mathbb{R}^6 ,

$$\begin{aligned} & \int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_t(dx_1 dv_1) \\ & = \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \int_{A_{\mathbf{k}_n \sigma_n}(t)} \varphi(z_1^F(t)) \mu_0^{n+1}(dz_{n+1}) \quad (23) \end{aligned}$$

where $\mathbf{z}^F(t, \mathbf{z}_{n+1}, \mathbf{k}_n, \sigma_n)$ is the forward Boltzmann–Enskog flow, $\mu_0(dx_1 dv_1)$ on \mathbb{R}^6 is any finite Borel measure and $\mu_0^n(d\mathbf{z}_n) := \mu_0(dz_1) \dots \mu_0(dz_n)$. We rewrite here the integration variables $\zeta(0)$ as \mathbf{z}_{n+1} , and $\zeta_1^F(t)$ as $z_1^F(t) = z_1^F(t, \mathbf{z}_{n+1}, \mathbf{k}_n, \sigma_n)$.

3.1 Pathologies

It may arise an ambiguity in this definition if the μ_0^{n+1} -measure of the boundary $\partial A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ of the region $A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ is not vanishing. Recall that $A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ is the set of the initial $n + 1$ -particle configurations leading to the tree $(\mathbf{k}_n, \boldsymbol{\sigma}_n)$. So, $\partial A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ is the set of the initial $n + 1$ -particle configurations that, depending on small perturbation, may realize or not the tree $(\mathbf{k}_n, \boldsymbol{\sigma}_n)$. A configuration \mathbf{z}_{n+1} belongs to $\partial A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ in several cases.

The first one corresponds to an initial configuration leading to a collision of the particles 1 and 2 exactly at the final instant t .

If a configuration leading to a collision at the instant t has a positive μ_0 -measure, then we need to consider either $t - \eta$ or $t + \eta$ instead. For this reason, we may demand (23) to be satisfied not for all t but for almost all t .

The second case when $\mathbf{z}_{n+1} \in \partial A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}(t)$ corresponds to initial configurations leading, in the forward Boltzmann–Enskog flow, to so called grazing collisions (collisions with $\omega \cdot (v - v_1) = 0$ in (2)). However, since we are interested in initial data of the form (3) for $t = 0$ also such pathology can be avoided by simply using that the initial configuration does not deliver grazing collisions in a finite time. In fact the set of such configurations is of full Lebesgue measure.

The previous pathologies depend on the hard-sphere dynamics, but there is also a pathology depending on the structure of Eq. (23). We illustrate it by means of an example. Consider the case $N = 2$ with initial measure

$$\mu_0(d\zeta_1 d\zeta_2) = \frac{1}{2}(\delta(\zeta_1 - z_1) + \delta(\zeta_2 - z_2))d\zeta_1 d\zeta_2$$

and with initial state (z_1, z_2) leading to a collision in the time $(0, t)$. If we compute the terms in the expansion relative to $n = 0, 1$, we easily recover the time evolved measure μ_t . This means that particle 2 is created in some definite instant t_1 , to fit with the initial configuration. However, as pointed out in [19], there are other non vanishing contributions. For instance particle 3 can be created by particle 2 with $\sigma_2 = -$ at time $t_1 - 0$. The initial contribution is

$$\delta(\zeta_1 - z_1)\delta(\zeta_2 - z_2)\delta(\zeta_3 - z_1) = \delta(\zeta_1 - z_1)\delta(\zeta_2 - z_2)\delta(\zeta_3 - \zeta_1).$$

Furthermore, an arbitrary number of branches with $\sigma_i = -, i > 1$ can be created accumulating at the first node, see Fig. 5. In order to prevent such an unphysical event, we introduce next a suitable notion of measure valued solution.

3.2 Regularization via time separation

In order to overcome the pathologies discussed above, we modify definition (23) by setting

$$\begin{aligned} & \int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_t(dx_1 dv_1) \\ &= \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\boldsymbol{\sigma}_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \lim_{\varepsilon \rightarrow 0^+} \int_{A_{\mathbf{k}_n, \boldsymbol{\sigma}_n}^\varepsilon(t)} \varphi(z_1^F(t)) \mu_0^{n+1}(d\mathbf{z}_{n+1}). \end{aligned} \quad (24)$$

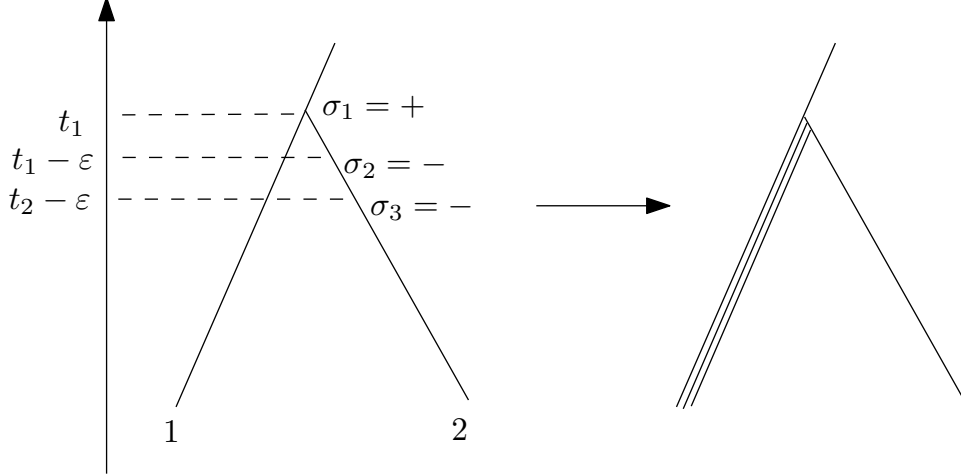


Figure 5: Initial configuration $\delta(\zeta_1 - z_1)\delta(\zeta_2 - z_2)\delta(\zeta_3 - z_1)\delta(\zeta_4 - z_1)\cdots$.

The difference between (23) and (24) consists in the introduction of the parameter ε and in the replacement of $A_{\mathbf{k}_n\sigma_n}(t)$ by $A_{\mathbf{k}_n\sigma_n}^\varepsilon(t)$ defined by

$$A_{\mathbf{k}_n\sigma_n}^\varepsilon(t) = A_{\mathbf{k}_n\sigma_n}(t) \setminus S_{\mathbf{k}_n\sigma_n}^\varepsilon(t),$$

where the set $S_{\mathbf{k}_n\sigma_n}^\varepsilon(t)$ consists of all the elements \mathbf{z}_{n+1} delivering, in the Boltzmann–Enskog forward flow, the event in which two particles, born from the same progenitor, are created at times t_i, t_j , such that $|t_i - t_j| \leq \varepsilon$. In other words, creations of particles from the same branch are time separated by $\varepsilon > 0$. Clearly, this avoids the main pathology envisaged in the previous section.

We take Equation (24) as definition of ‘regularized series solution’ for a given initial measure μ_0 . We will apply this notion only to initial measures which are empirical distributions, namely of the form (3) at time 0. Notice, however, that the regularized series solution makes sense for any initial μ_0 .

Remark 3 *One could have defined the time separation on all the nodes of a fully ordered tree. This would not be good for our purpose, since simultaneous creations from different branches of a tree play a crucial role in the reconstruction of the hard-sphere dynamics (see Section 4.2 below).*

A crucial property of the weak series solution is the semigroup property which we are going to illustrate.

3.3 Semigroup property

Proposition 2 (Semigroup property) *Let μ_0 be such that configurations leading to grazing collisions have zero μ_0^{n+1} -measure for all n, \mathbf{k}_n , and σ_n . Let also $t > 0$ and $\tau \in (0, t)$ be such that initial configurations leading to collisions at the instants τ or t have zero μ_0^{n+1} -measure for all n, \mathbf{k}_n , and σ_n . If the following*

equalities are satisfied:

$$\begin{aligned} & \int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_\tau(dx_1 dv_1) \\ &= \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \lim_{\varepsilon \rightarrow 0^+} \int_{A_{\mathbf{k}_n \sigma_n}^\varepsilon(\tau)} \varphi(z_1^F(\tau)) \mu_0^{n+1}(d\mathbf{z}_{n+1}), \end{aligned} \quad (25)$$

$$\begin{aligned} & \int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_t(dx_1 dv_1) \\ &= \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \lim_{\varepsilon \rightarrow 0^+} \int_{A_{\mathbf{k}_n \sigma_n}^\varepsilon(t-\tau)} \varphi(z_1^F(t-\tau)) \mu_\tau^{n+1}(d\mathbf{z}_{n+1}), \end{aligned} \quad (26)$$

then equality (24) is also satisfied. Conversely, if (24) is satisfied for t and τ , then (25) is also satisfied.

Proof. Rewrite the integral in (26) as

$$\begin{aligned} & \int_{A_{\mathbf{k}_n \sigma_n}^\varepsilon(t-\tau)} \varphi(z_1^F(t-\tau, \mathbf{z}_{n+1}, \mathbf{k}_n, \sigma_n)) \mu_\tau^{n+1}(d\mathbf{z}_{n+1}) \\ &= \int_{\mathbb{R}^6} \mu_\tau(dz_1) \dots \int_{\mathbb{R}^6} \mu_\tau(dz_{n+1}) \psi(t-\tau, z_1, \dots, z_{n+1}, \mathbf{k}_n, \sigma_n), \end{aligned} \quad (27)$$

where

$$\psi(t-\tau, \mathbf{z}_{n+1}, \mathbf{k}_n, \sigma_n) = \varphi(z_1^F(t-\tau, \mathbf{z}_{n+1}, \mathbf{k}_n, \sigma_n)) \chi_{A_{\mathbf{k}_n \sigma_n}^\varepsilon(t-\tau)}(\mathbf{z}_{n+1}),$$

and $\chi_{\mathcal{A}}$ is a characteristic function of a set \mathcal{A} .

Firstly, we give a heuristic proof of the proposition, then we give a formal proof. We apply formula (25) $n+1$ times. Each n -tuple \mathbf{k}_n in expansion (26) corresponds to one tree for the interval $[\tau, t)$. Applications of (25) to (27) give $n+1$ trees $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$, which are, graphically, continuations of the final points of the tree \mathbf{k}_n (see Fig. 6). So, the composition of the tree \mathbf{k}_n with the trees $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$ yields a new tree \mathbf{K}_N , where $N = n + m_1 + \dots + m_{n+1}$. The Boltzmann–Enskog backward flows produced by the trees $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$ for the time interval $[0, \tau]$ together constitute a continuation of the Boltzmann–Enskog backward flow produced by the tree \mathbf{k}_n . Their composition yields the Boltzmann–Enskog backward flow produced by the tree \mathbf{K}_N . Conversely, the Boltzmann–Enskog forward flow produced by the tree \mathbf{k}_n is a continuation of the n -tuple of the Boltzmann–Enskog forward flows produced by the trees $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$. Their composition also yields the Boltzmann–Enskog forward flow produced by the tree \mathbf{K}_N .

From the graphical representation, one can understand that the summations over all \mathbf{k}_n and over all $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$ gives the summation over all joint trees \mathbf{K}_N for the whole interval $[0, t]$.

Now we give a formal proof of the proposition. After the application of (25) to

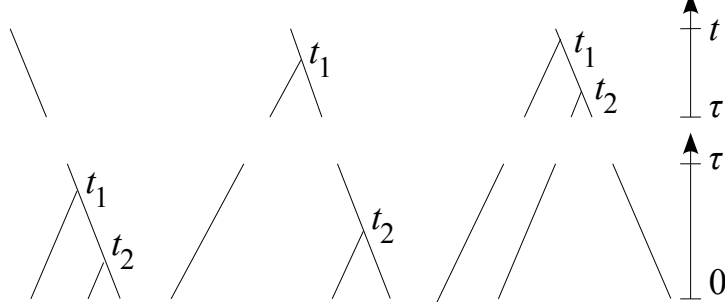


Figure 6: Sum of compositions of trees.

(27), a generic term is

$$\left(\frac{\lambda}{a^2}\right)^N \prod_{i=1}^N \Sigma_i \lim_{\varepsilon \rightarrow 0} \int_{A_{\mathbf{k}_{m_1}^1 \sigma_{m_1}^1}^\varepsilon(\tau) \times \dots \times A_{\mathbf{k}_{m_{n+1}}^{n+1} \sigma_{m_{n+1}}^{n+1}}^\varepsilon(\tau)} \psi(t - \tau, \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N), \mathbf{k}_n, \sigma_n) \mu_0^{N+1}(d\mathbf{z}_{N+1}), \quad (28)$$

where $\Sigma_i = \pm$ and

$$\begin{aligned} & \psi(t - \tau, \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N), \mathbf{k}_n, \sigma_n) \\ &= \varphi(z_1^F(t - \tau, \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N), \mathbf{k}_n, \sigma_n)) \\ & \quad \times \chi_{A_{\mathbf{k}_n \sigma_n}^\varepsilon(t - \tau)}(\mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N)). \end{aligned} \quad (29)$$

Note that, in (28), we have replaced the product of limits $\lim_{\varepsilon_q \rightarrow 0}$, $q = 1, \dots, n+1$ (running over the final points of the tree \mathbf{k}_n), with a single limit $\lim_{\varepsilon \rightarrow 0}$. The result is indeed independent on the precise way in which the regularization is removed in the different subtrees.

In the first factor in the right-hand side of (29), we see a composition of two Boltzmann–Enskog forward flows: for the interval $[0, \tau]$ (determined by the “bottom trees” $\mathbf{k}_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1}$) and for the interval $[\tau, t]$ (determined by the “top tree” \mathbf{k}_n). We have

$$z_1^F(t - \tau, \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N), \mathbf{k}_n, \sigma_n) = z_1^F(t, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N).$$

The characteristic function in (29) means that, actually, the integration in (28) takes place over initial configurations in

$$A_{\mathbf{k}_{m_1}^1 \sigma_{m_1}^1}^\varepsilon(\tau) \times \dots \times A_{\mathbf{k}_{m_{n+1}}^{n+1} \sigma_{m_{n+1}}^{n+1}}^\varepsilon(\tau)$$

leading to configurations in $A_{\mathbf{k}_n \sigma_n}^\varepsilon(t - \tau)$ at the instant τ , i.e., over the set

$$\left\{ \mathbf{z}_{N+1} \in A_{\mathbf{k}_{m_1}^1 \sigma_{m_1}^1}^\varepsilon(\tau) \times \dots \times A_{\mathbf{k}_{m_{n+1}}^{n+1} \sigma_{m_{n+1}}^{n+1}}^\varepsilon(\tau) \mid \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N) \in A_{\mathbf{k}_n \sigma_n}^\varepsilon(t - \tau) \right\}. \quad (30)$$

Consider another set:

$$\{\mathbf{z}_{N+1} \in A_{\mathbf{K}_N \Sigma_N}^\varepsilon(t) \mid \mathbf{z}_{n+1}^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N) \in A_{\mathbf{k}_n \sigma_n}^\varepsilon(t - \tau)\} = B_{\mathbf{K}_N \Sigma_N t}^{\mathbf{k}_n \sigma_n t - \tau; \varepsilon}. \quad (31)$$

Since, for a fixed (\mathbf{k}_n, σ_n) , the ‘‘bottom trees’’

$$(\mathbf{k}_{m_1}^1 \sigma_{m_1}^1, \dots, \mathbf{k}_{m_{n+1}}^{n+1} \sigma_{m_{n+1}}^{n+1})$$

and the joint tree (\mathbf{K}_N, Σ_N) are in a one-to-one correspondence, sets (30) and (31) coincide if $\varepsilon = 0$.

If $\varepsilon > 0$, then these sets slightly differ. Namely, set (30) does not demand the time separation between subsequent collisions of the same particle in a neighbourhood of the instant τ . Consider, for example, the second composition of trees on Fig. 6, where $t_1 \in [\tau, t]$ and $t_2 \in [0, \tau]$. There is no demand of time separation between t_1 and t_2 in this composition: both t_1 and t_2 are allowed to be arbitrary close to τ . However, by assumption, the μ_0^{N+1} -measure of initial configurations leading to collisions in a ε -neighbourhood of τ tends to zero for all triples $(N, \mathbf{K}_N, \Sigma_N)$. Hence, in the limit $\varepsilon \rightarrow 0$, the integrals over set (30) and over set (31) with respect to the measure μ_0^{N+1} coincide.

Thus, the right-hand side of (26) can be written as

$$\begin{aligned} & \sum_{n=0}^{\infty} \sum_{m_1=0}^{\infty} \dots \sum_{m_{n+1}=0}^{\infty} \left(\frac{\lambda}{a^2} \right)^N \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \\ & \sum_{\mathbf{k}_{m_1}^1 \in \mathcal{K}_{m_1}} \sum_{\sigma_{m_1}^1 \in \{\pm\}^{m_1}} \dots \sum_{\mathbf{k}_{m_{n+1}}^{n+1} \in \mathcal{K}_{m_{n+1}}} \sum_{\sigma_{m_{n+1}}^{n+1} \in \{\pm\}^{m_{n+1}}} \prod_{i=1}^N \Sigma_i \lim_{\varepsilon \rightarrow 0} \\ & \int_{B_{\mathbf{K}_N \Sigma_N t}^{\mathbf{k}_n \sigma_n t - \tau; \varepsilon}} \varphi(z_1^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N)) \mu_0^{N+1}(d\mathbf{z}_{N+1}). \quad (32) \end{aligned}$$

The summation over $(m_1, \mathbf{k}_{m_1}^1, \sigma_{m_1}^1, \dots, m_{n+1}, \mathbf{k}_{m_{n+1}}^{n+1}, \sigma_{m_{n+1}}^{n+1})$ can be replaced by the summation over $(N, \mathbf{K}_N, \Sigma_N)$, because, as we said before, they are in one-to-one correspondence for fixed $(n, \mathbf{k}_n, \sigma_n)$. Hence, (32) can be rewritten as

$$\begin{aligned} & \sum_{N=0}^{\infty} \left(\frac{\lambda}{a^2} \right)^N \sum_{\mathbf{K}_N \in \mathcal{K}_N} \sum_{\Sigma_N \in \{\pm\}^N} \sum_{n=0}^{\infty} \sum_{\mathbf{k}_n \in \mathcal{K}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^N \Sigma_i \\ & \times \lim_{\varepsilon \rightarrow 0} \int_{B_{\mathbf{K}_N \Sigma_N t}^{\mathbf{k}_n \sigma_n t - \tau; \varepsilon}} \varphi(z_1^F(\tau, \mathbf{z}_{N+1}, \mathbf{K}_N, \Sigma_N)) \mu_0^{N+1}(d\mathbf{z}_{N+1}). \quad (33) \end{aligned}$$

For every triple $(N, \mathbf{K}_N, \Sigma_N)$,

$$\bigcup_{n=0}^{\infty} \bigcup_{\mathbf{k}_n \in \mathcal{K}_n} \bigcup_{\sigma_n \in \{\pm\}^n} B_{\mathbf{K}_N \Sigma_N t}^{\mathbf{k}_n \sigma_n t - \tau; \varepsilon} = A_{\mathbf{K}_N \Sigma_N}^\varepsilon(t),$$

hence the summation over $(n, \mathbf{k}_n, \boldsymbol{\sigma}_n)$ in (33) gives the integral over $A_{\mathbf{K}_N \boldsymbol{\Sigma}_N}^\varepsilon(t)$:

$$\begin{aligned} \int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_t(dx_1 dv_1) &= \sum_{N=0}^{\infty} \left(\frac{\lambda}{a^2} \right)^N \sum_{\mathbf{K}_N \in \mathcal{K}_N} \sum_{\boldsymbol{\Sigma}_N \in \{\pm\}^N} \prod_{i=1}^N \Sigma_i \\ &\quad \times \lim_{\varepsilon \rightarrow 0} \int_{A_{\mathbf{K}_N \boldsymbol{\Sigma}_N}^\varepsilon(t)} \varphi(z_1^F(t, \mathbf{z}_{N+1}, \mathbf{K}_N, \boldsymbol{\Sigma}_N)) \mu_0^{N+1}(d\mathbf{z}_{N+1}), \end{aligned}$$

which coincides with (24).

4 Microscopic solutions of the Boltzmann–Enskog equation

4.1 Main result

We are going to prove that a measure of form (3) is a weak series solution of the Boltzmann–Enskog equation, i.e., satisfies (24). We assume that the initial configuration $\mathbf{z}^0 = (z_1^0, \dots, z_N^0)$ is such that configurations $(z_i^0)_{i \in \mathcal{I}_n}$, for all non-empty $\mathcal{I}_n \subset \{1, \dots, N\}$, lead to a well-defined hard-sphere motion and do not lead to grazing collisions. Also, for simplicity, let us assume that the initial configuration \mathbf{z}^0 does not lead to simultaneous collisions of different pairs of hard spheres. As previously recalled, the set of initial configurations satisfying these conditions has full measure.

Theorem 4.1 *Let $\lambda = Na^2$. Under the above assumptions on \mathbf{z}^0 , the empirical measure (3) is a weak series solution of the Boltzmann–Enskog equation, i.e., it satisfies (24).*

Proof. Denote by $\mathbb{T}_n(s)$, $s \in [0, t]$ the n -particle hard sphere flow. As before, denote $\mathbf{z}(s) = \mathbb{T}_N(s)\mathbf{z}^0$. Let t be such that the configurations $(z_i^0)_{i \in \mathcal{I}_n}$ do not lead to collisions at the instant t .

Let us partition the interval $[0, t)$ in a sequence of intervals $[\theta_j, \theta_{j+1})$, $j = 0, \dots, S-1$, $0 = \theta_0 < \theta_1 < \dots < \theta_S = t$ with the following properties:

- (i) In each interval (θ_j, θ_{j+1}) , at most one collision in the hard sphere dynamics starting from \mathbf{z}^0 occurs. There are no collision at the instants θ_j , $j = 1, \dots, S$.
- (ii) Let the particles l and m collide in the interval $[\theta_j, \theta_{j+1})$. Then both flows

$$\mathbb{T}_{N-1}(s) (z_i(\theta_j))_{i \in \{1, \dots, l-1, l+1, \dots, N\}}, \quad s \in [0, \theta_{j+1} - \theta_j],$$

and

$$\mathbb{T}_{N-1}(s) (z_i(\theta_j))_{i \in \{1, \dots, m-1, m+1, \dots, N\}}, \quad s \in [0, \theta_{j+1} - \theta_j],$$

are free.

Due to the semigroup property (Proposition 2), it is sufficient to prove (24) for a single interval, say, $[0, \theta_1)$.

The left-hand side of (24) is, for all $s \in [0, \theta_1]$

$$\int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_s(dx_1 dv_1) = \frac{1}{N} \sum_{i=1}^N \varphi(x_i(s), v_i(s)). \quad (34)$$

Denote the terms on the right-hand side of (24) as $\sum_{n=0}^{\infty} \Phi_n$. The $n = 0$ term is

$$\Phi_0 = \int_{\mathbb{R}^6} \varphi(x_1 + v_1 s, v_1) \mu_0(dx_1 dv_1) = \frac{1}{N} \sum_{i=1}^N \varphi(x_i^0 + v_i^0 s, v_i^0).$$

If there are no collisions in the interval $[0, s)$, then $x_i(s) = x_i^0 + v_i^0 s$, $v_i(s) = v_i^0$, and Φ_0 coincides with (34). Moreover, the higher-order terms vanish since $A_{\mathbf{k}_n, \sigma_n}^\varepsilon(s)$ does not intersect with $\text{supp } \mu_0 = \{z_i^0\}_{i=1}^N$ in this case. So, (3) obviously satisfies (24) in this interval.

Let now particles l and m collide at an instant $\tau \in (0, \theta_1)$. By our hypotheses, all the other particles move freely. Then

$$\begin{aligned} x_l(s) &= x_l^0 + v_l^0 \tau + v'_l(s - \tau), \\ x_m(s) &= x_m^0 + v_m^0 \tau + v'_m(s - \tau), \\ x_i(s) &= x_i^0 + v_i^0 s, \quad i \neq l, m, \end{aligned}$$

where v'_l and v'_m are related to v_l^0 and v_m^0 by (2). Considering the first-order terms, we have $\mathbf{k}_1 = 1$ (the only possibility) and

$$A_{\mathbf{k}_1, \sigma_1}^\varepsilon \cap \text{supp } \mu_0^2 = \{(z_l^0, z_m^0), (z_m^0, z_l^0)\}$$

for every $\sigma_1 = \pm$. The first-order term in the right-hand side of (24) is then

$$\begin{aligned} \Phi_1 &= N \sum_{\sigma_1 \in \{\pm\}} \sigma_1 \lim_{\varepsilon \rightarrow 0} \int_{A_{\mathbf{k}_1, \sigma_1}^\varepsilon(s)} \varphi(z_1^F(s, z_1, z_2, k_1, \sigma_1)) \mu_0^2(dz_1 dz_2) \\ &= \frac{1}{N} [\varphi(z_1^F(s, (z_l^0, z_m^0), \mathbf{k}_1, +)) + \varphi(z_1^F(s, (z_m^0, z_l^0), \mathbf{k}_1, +)) \\ &\quad - \varphi(z_1^F(s, (z_l^0, z_m^0), \mathbf{k}_1, -)) - \varphi(z_1^F(s, (z_m^0, z_l^0), \mathbf{k}_1, -))] . \end{aligned}$$

In the case $\sigma_1 = +$, the Boltzmann–Enskog forward flow coincides with the hard sphere dynamics, i.e.,

$$\begin{aligned} z_1^F(s, (z_l^0, z_m^0), \mathbf{k}_1, +) &= z_l(s) = (x_l^0 + v_l^0 \tau + v'_l(s - \tau), v'_l), \\ z_1^F(s, (z_m^0, z_l^0), \mathbf{k}_1, +) &= z_m(s) = (x_m^0 + v_m^0 \tau + v'_m(s - \tau), v'_m). \end{aligned}$$

In the case $\sigma_1 = -$, the Boltzmann–Enskog forward flow for the particle 1 coincides with the free dynamics of the particle 1, i.e.,

$$\begin{aligned} z_1^F(s, (z_l^0, z_m^0), \mathbf{k}_1, -) &= (x_l^0 + v_l^0 s, v_l), \\ z_1^F(s, (z_m^0, z_l^0), \mathbf{k}_1, -) &= (x_m^0 + v_m^0 s, v_m). \end{aligned}$$

Hence,

$$\Phi_1 = \frac{1}{N} [\varphi(x_l(s), v_l(s)) + \varphi(x_m(s), v_m(s)) - \varphi(x_l^0 + v_l^0 s, v_l^0) - \varphi(x_m^0 + v_m^0 s, v_m^0)],$$

so that $\Phi_0 + \Phi_1$ is equal to (34).

The higher-order terms vanish since $A_{\mathbf{k}_n \sigma_n}^\varepsilon(s)$ for $n \geq 2$ does not intersect with $\text{supp } \mu_0$. Consider, for example, $n = 2$. Configurations like (z_i^0, z_j^0, z_r^0) with $i \neq j \neq r$ for $\sigma_2 = (+, +)$ do not lead to two subsequent collisions, since the Boltzmann–Enskog forward flow coincides with the hard sphere dynamics for this choice of σ_2 . But, by property (i) of the intervals, hard spheres suffer at most one collision on the interval $[0, \theta_1)$. The same configurations for $\sigma_2 = (+, -), (-, +), (-, -)$ do not lead to two collisions by property (ii): neither particle l ignoring particle m collides with another particle nor particle m ignoring particle l collides with another particle; other particles move freely. Configurations like $(z_l^0, z_m^0, z_m^0) \in \text{supp } \mu_0^3$ could be interpreted as configurations leading to two collisions: the first particle collides with the second and the third particles at the same instant τ . However, by definition of $A_{\mathbf{k}_n \sigma_n}^\varepsilon(s)$, the subsequent collisions of the same particle should be ε -separated in time.

Thus, (3) satisfies (24) in the interval $[0, \theta_1)$ in the case of a single collision in this interval. This concludes the proof of the theorem.

Remark 4 *Note that Proposition 1, adapted to the present context, guarantees the convergence of series (24) only for small λ . However, in case of microscopic solutions, the series has only a finite number of non-vanishing terms, by construction, so that it converges for arbitrary large $\lambda = Na^2$.*

4.2 Recollisions vs. contractions

There is another and more natural way to describe the hard-sphere dynamics for a microscopic state in terms of a series expansion.

The j -particle marginals associated to a time evolving particle configuration $\mathbf{z}_N(t) = \mathbb{T}_N(t)\mathbf{z}_N(0) = \{\bar{z}_1(t), \dots, \bar{z}_N(t)\}$ are defined by

$$\Delta_j(\mathbf{z}_j, t) = \frac{1}{N(N-1)\dots(N-j+1)} \sum_{\substack{i_1, \dots, i_j \\ i_a \neq i_b}} \prod_{s=1}^j \delta(z_s - \bar{z}_{i_s}(t)) \quad (35)$$

where $\mathbf{z}_j = (z_1 \dots z_j)$.

For $j = 1$ we recover the time-evolved empirical distribution (3).

In [19] it has been proved that (35) satisfies the following series expansion (BBGKY hierarchy)

$$\begin{aligned} \Delta_j(t) &= \mathcal{S}_{1\dots j}^{int} f_{0,j} + \sum_{n=1}^{N-j} a^{2n} (N-j)(N-j-1)\dots(N-j-n+1) \\ &\quad \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \\ &\quad \mathcal{S}_{1\dots j}^{int}(t-t_1) \mathcal{C}_{j+1} \mathcal{S}_{1\dots j+1}^{int}(t_1-t_2) \dots \mathcal{C}_{j+n} \mathcal{S}_{1\dots j+n}^{int}(t_n) \Delta_{0,j+n}, \end{aligned} \quad (36)$$

where

$$\mathcal{S}_{1\dots j}^{int}(t) F(\mathbf{z}_j) = F(\mathbb{T}_j(-t)\mathbf{z}_j) = F(\mathbf{z}_j(-t))$$

and \mathbb{T}_j is the j -particle interacting flow.

The validity of the above expansion, for $j = 1$ can be compared with the one of the Boltzmann–Enskog equation, which we rewrite here as

$$\mu_t = \mathcal{S}_1(t)\mu_0 + \sum_{n=1}^{\infty} \lambda^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \mathcal{S}_1(t-t_1)\mathcal{C}_2 \dots \mathcal{C}_{1+n}\mathcal{S}_{1\dots 1+n}(t_n)\mu_{0,1+n}, \quad (37)$$

where $\mu_{0,j} = \mu_0^{\otimes j}$. Eq.(37) has to be interpreted according to the notion of weak series solution discussed in this paper.

The right-hand sides of (36) for $j = 1$ and (37) must coincide, being identical the left hand sides. How is this possible?

First, observe that

$$\mu_{0,j} = \frac{N(N-1)(N-2)\dots(N-j+1)}{N^j} \Delta_{0,j}.$$

Note that the above identity holds on the physical phase space only, namely on the set of configurations for which $|x_k - x_\ell| > a$ for all $k \neq \ell$. Furthermore we take into account that $\lambda = a^2 N$ and that the the sum \sum^{N-1} can be replaced by \sum^∞ by adding vanishing terms. Then we conclude that the two series are identical but for the fact that $\mathcal{S}^{int}(t) \neq \mathcal{S}(t)$. More precisely, the backward flow $\mathcal{S}^{int}(t)$ describes also the collisions among the particles already created. Such interactions are usually called ‘recollisions’. In contrast, $\mathcal{S}(t)$ is just the free flow which implies that, once two particles are created, if they arrive at distance a (necessarily with outgoing velocities), they go ahead freely by backward overlapping.

More precisely, [19] proves the validity of a representation of the form:

$$\int_{\mathbb{R}^6} \varphi(x_1, v_1) \mu_t(dx_1 dv_1) = \sum_{n=0}^{\infty} \left(\frac{\lambda}{a^2}\right)^n \sum_{\mathbf{r}_n} \sum_{\sigma_n \in \{\pm\}^n} \prod_{i=1}^n \sigma_i \times \int_{\bar{A}_{\mathbf{r}_n \sigma_n}(t)} \varphi(z_1^{FI}(t, \mathbf{z}_{n+1}, \mathbf{r}_n, \sigma_n)) \mu_0^{\otimes(n+1)}(d\mathbf{z}_{n+1}), \quad (38)$$

where $z_1^{FI}(t, \mathbf{z}_{n+1}, \mathbf{r}_n, \sigma_n)$ is the interacting forward flow, taking into account the recollisions. Here there is no necessity of time separation and, as we have already illustrated, the sum over the fully ordered trees can be replaced by the sum over the partially ordered trees.

Remark 5 *The above equation must be further clarified (see [19]). In fact, in contrast with the Boltzmann–Enskog flow, the corresponding (\mathbf{r}_n, σ_n) -dependent map (‘interacting backward flow’)*

$$(x_1, v_1, \mathbf{t}_n, \boldsymbol{\omega}_n, \mathbf{v}_n) \mapsto \zeta^{BI}(0), \quad (39)$$

of which $\bar{A}_{\mathbf{r}_n \sigma_n}(t)$ is the image, is not globally invertible, but only locally. However (38) makes sense if we assume that φ has small enough support. We shall make this assumption in the discussion that follows.

The two representations (38) and (24) provide indeed the same result.

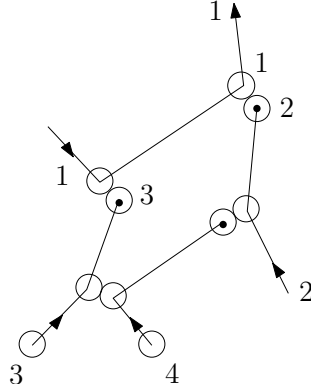
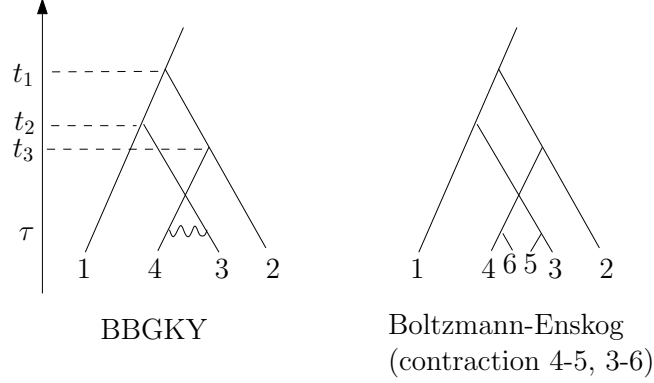


Figure 7:

Consider the following simple example with $N = 4$. The tree associated to (38) is given by $\mathbf{r}_3 = \{1, 1, 2\}$ while the one associated to the Boltzmann–Enskog expansion is $\mathbf{k}_6 = \{2, 1, 1, 1, 0, 0\}$, see Fig. 7.

The wavy line of the first tree denotes that particles 3 and 4 recollide at some time $\tau \in (0, t_3)$ according, say, to the hard-sphere dynamics in the figure.

Such a recollision can be described as well in terms of the Boltzmann–Enskog flow, by a creation of two (fictitious) particles 5 and 6. Recalling that $\frac{\lambda}{a^2} = N = 4$, the 5-th order term of (24) is then equal to the 3-th order term of (38). Indeed the former is

$$\frac{1}{4}\varphi(\bar{z}_1(t)) \int \prod_{i=1}^6 dz_i \delta(z_1 - \bar{z}_1(0))\delta(z_2 - \bar{z}_2(0))\delta(z_3 - \bar{z}_3(0))\delta(z_4 - \bar{z}_4(0)) \\ \times \delta(z_5 - \bar{z}_4(0))\delta(z_6 - \bar{z}_3(0)) = \frac{1}{4}\varphi(\bar{z}_1(t))$$

while the second is

$$\frac{1}{4}\varphi(\bar{z}_1(t)) \int \prod_{i=1}^4 dz_i \delta(z_1 - \bar{z}_1)\delta(z_2 - \bar{z}_2)\delta(z_3 - \bar{z}_3)\delta(z_4 - \bar{z}_4) = \frac{1}{4}\varphi(\bar{z}_1(t)) .$$

Summarizing we see that the integration in $\prod_{i=1}^6 dz_i$ follows by a reduction of the computation at time zero by means of the map (14) associated to the Boltzmann–

Enskog backward flow, while the integration $\prod_{i=1}^4 dz_i$ follows by the corresponding map associated to the interacting backward flow.

This example shows also that a full time separation cannot work as regularization, because it cannot describe recollisions which, in the Boltzmann–Enskog expansion, are given by simultaneous creations of two particles, contracted with previously existing particles of the backward flow.

Remark 6 *The previous argument shows that Eq. (38) could be derived by assuming (24) and vice versa.*

4.3 Conclusions

The presented way of giving a rigorous sense to the microscopic solutions of the Boltzmann–Enskog equation appears to be the most natural one, in comparison to the previously proposed variants [23, 24, 25, 26], since it does not involve regularizations of delta functions, but gives direct sense to weak solutions of the Boltzmann–Enskog equation by means of a notion of series solution. Here we have introduced a series expansion that involves only partial chronological ordering of collisions. The result is recovered by the time separation of collisions corresponding to this partial order. Thus, the Boltzmann–Enskog equation, which is known to describe irreversible dynamics and entropy production, contains also solutions corresponding to the reversible microscopic dynamics of hard spheres.

Formula (24) for weak series solutions is not very handable for practical purposes, but reveals a relation of solutions of the Boltzmann–Enskog equation with the hard sphere dynamics.

Acknowledgments

The work of A.T. was supported by the grant of the President of the Russian Federation (project MK-2815.2017.1). S.S. acknowledges support from DFG grant 269134396.

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