



**HAL**  
open science

# On the cardinality of collisional clusters for hard spheres at low density

Mario Pulvirenti, Sergio Simonella

► **To cite this version:**

Mario Pulvirenti, Sergio Simonella. On the cardinality of collisional clusters for hard spheres at low density. *Discrete and Continuous Dynamical Systems - Series A*, 2021. hal-02614992v2

**HAL Id: hal-02614992**

**<https://hal.science/hal-02614992v2>**

Submitted on 14 Apr 2021

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# On the cardinality of collisional clusters for hard spheres at low density

M. Pulvirenti<sup>1</sup> and S. Simonella<sup>2</sup>

1. DIPARTIMENTO DI MATEMATICA, UNIVERSITÀ DI ROMA LA SAPIENZA  
PIAZZALE ALDO MORO 5, 00185 ROME – ITALY, AND  
INTERNATIONAL RESEARCH CENTER M&MOCS, UNIVERSITÀ DELL'AQUILA,  
PALAZZO CAETANI, 04012 CISTERNA DI LATINA – ITALY.

2. UMPA UMR 5669 CNRS, ENS DE LYON  
46 ALLÉE D'ITALIE, 69364 LYON CEDEX 07 – FRANCE

**Abstract.** We resume the investigation, started in [2], of the statistics of backward clusters in a gas of  $N$  hard spheres of small diameter  $\varepsilon$ . A backward cluster is defined as the group of particles involved directly or indirectly in the backwards-in-time dynamics of a given tagged sphere. We obtain an estimate of the average cardinality of clusters with respect to the equilibrium measure, global in time, uniform in  $\varepsilon$ ,  $N$  for  $\varepsilon^2 N = 1$  (Boltzmann-Grad regime).

**Keywords.** Hard spheres; low-density gas; Boltzmann equation; backward cluster.

# 1 Introduction

Boltzmann's equation, its actual relation with particle systems and higher order density corrections have led, through the years, to several mathematical questions around collisions in hard-sphere type models. A famous example is the problem of counting the number of collisions in a group of hard balls [16]. This is of interest in its own and it is a problem of great geometric complexity [26, 5, 22]. More closely related to the kinetic theory of gases is the analysis of the statistical (average) behaviour of collision sequences, for a finite subgroup of particles in a large (eventually infinite) system of hard spheres. At low density, if particle "1" undergoes  $k$  collisions, it will typically interact with  $k$  different spheres. Collecting these "fresh" particles, together with the fresh particles encountered by them, and so on, we arrive to a natural notion of "cluster of influence", to be associated to the particle 1. These clusters have both theoretical and applied interest and they are involved in the control of dynamical correlations [2, 20, 4]. Our goal is to derive an estimate on the cardinality of collisional clusters, uniform in the low-density (Boltzmann-Grad) limit. The estimate is valid globally in time, both with respect to an equilibrium measure, or with respect to a nonequilibrium measure with strong boundedness properties. Note that the control of the size of backward clusters implies the absence of very large chains of collisions, which could prevent the propagation of chaos in the Boltzmann-Grad limit.

The definition of cluster is given in the next section. Our main result (Theorem 2.1) is presented in Section 2, while Section 2.1 discusses the difficulties encountered in controlling the size of clusters. Section 3 is devoted to the proof of the theorem.

In this paper we consider hard-sphere systems, however we believe that our results can be extended to particle systems interacting via suitable (say, repulsive) short-range potentials, by using approach and techniques inspired from [12, 14, 9, 19].

## 1.1 Backward and forward clusters

Consider a system of  $N$  identical hard spheres of diameter  $\varepsilon > 0$  moving in the three-dimensional space. To fix the ideas we will confine the spheres to the torus  $\mathbb{T}^3 = [0, 2\pi)^3$  (although different boundary conditions might be considered). The spheres collide by means of the laws of elastic reflection [1]. A configuration of the system is  $Z_N = (z_1, \dots, z_N)$ , where  $z_i = (x_i, v_i) \in \mathbb{T}^3 \times \mathbb{R}^3$  are the position and the velocity of particle  $i$  respectively.

Given a particle, say particle 1, consider  $z_1(t, Z_N)$  its state (position and velocity) at time  $t$  for the initial configuration  $Z_N$ . We define the *backward cluster of particle 1* (at time  $t$  and for the initial configuration  $Z_N$ ) as the ordered set of particles with indices  $BC(1) \subset$

$I_N := \{1, 2, \dots, N\}$ , constructed in the following way. Going back in time starting from  $z_1(t, Z_N)$ , let  $i_1$  be the first particle colliding with 1. Next, considering the two particles 1 and  $i_1$ , let us go back in time up to the first collision of one particle of the pair with a new particle  $i_2$ . We iterate this procedure up to time 0. Then  $BC(1) := \{i_1, i_2, \dots, i_n\}$  with  $i_r \neq i_s$  for  $r \neq s$ .

In [2] we introduced and studied the problem of determining the time evolution of  $|BC(1)|$ , the cardinality of backward clusters. We showed that this hard task simplifies considerably in the Boltzmann-Grad limit [11], as one can resort to the Boltzmann equation to prove exponential growth. We also discussed the connection with the hierarchy of equations. At low density, dynamical observables admit a perturbative representation as ‘sums over backward clusters’. This is suggested, in particular, by a special representation of the solution to the Boltzmann equation, well known under the name of Wild sum [27, 2].

We point out here that a definition of *forward cluster*  $FC(1)$  can be given by the same identical procedure, just reversing the direction in time. Namely we start from  $z_1$  (configuration of particle 1 at time zero) and move up to  $z_1(t, Z_N)$ , drawing the forward cluster of influence. This notion may have a different applied interest as e.g. in the rate of spread of an epidemic [21]. In the present paper, we will focus on the backward cluster, although our results will be obviously true for forward clusters as well.

We may add to the previous definition an internal *structure*, by specifying the sequence of colliding pairs. To do this, we introduce binary tree graphs. A *n-collision tree*  $\Gamma_n$  is the collection of integers  $k_1, \dots, k_n$  such that

$$k_1 \in I_1, k_2 \in I_2, \dots, k_n \in I_n, \quad \text{where} \quad I_s = \{1, 2, \dots, s\}. \quad (1.1)$$

We say that the backward cluster  $BC(1)$  has structure  $\Gamma_n = (k_1, \dots, k_n)$  if  $|BC(1)| = n$  and the ordering of the collisions producing the cluster is specified by the tree. For a graphical representation, see the example in Figure 1.

Clearly, the collisions defining the backward cluster (involving a “new” particle) are not the only collisions showing up in the trajectory of the cluster. Collisions which do not involve a new particle are called *recollisions* (e.g. the collision between  $(i_2, i_3)$  in the figure).

Let now assign a probability density  $W_0^N$  symmetric in the exchange of particles, on the  $N$ -particle phase space,

$$\mathcal{M}_N := \left\{ Z_N \in (\mathbb{T}^3 \times \mathbb{R}^3)^N, \quad |x_i - x_j| > \varepsilon, \quad i \neq j \right\}. \quad (1.2)$$

In general, the measure is non-stationary and we denote by  $W^N(t)$  the time-evolved density. This is transported along the hard-sphere flow  $Z_N \rightarrow \Phi_N^t(Z_N)$ ,  $t > 0$ , precisely defined as

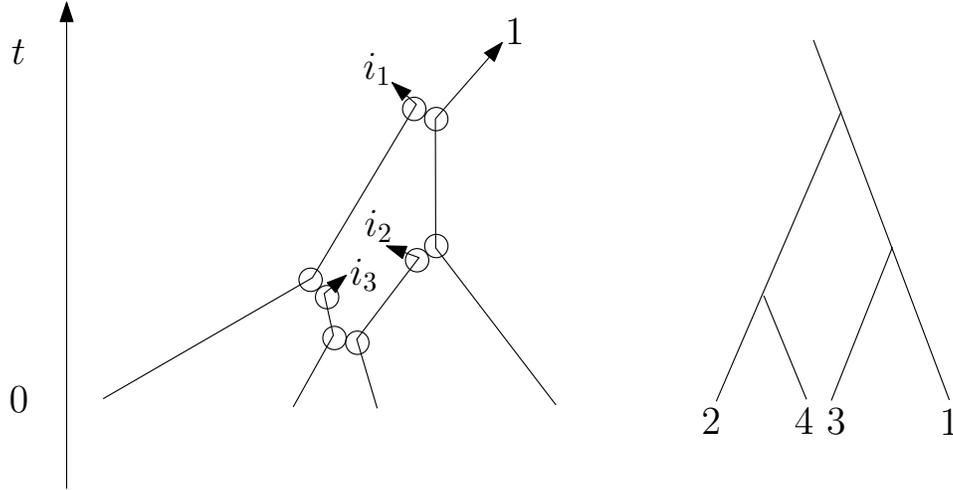


Figure 1: The trajectory of a backward cluster  $BC(1)$  at time  $t$  (of cardinality 3) is represented on the left. Its tree structure  $\Gamma_3 = (1, 1, 2)$  is given by the graph on the right.

follows. Given a time-zero configuration  $Z_N \in \mathcal{M}_N$ , each particle will move on a straight line with constant velocity between collisions; when two hard spheres collide with positions  $x_i, x_j$  at distance  $\varepsilon$ , normalized relative distance  $\omega = (x_i - x_j)/|x_i - x_j| = (x_i - x_j)/\varepsilon \in \mathbb{S}^2$  and incoming velocities  $v_i, v_j$  (i.e.  $(v_i - v_j) \cdot \omega < 0$ ), these are instantaneously transformed to outgoing velocities  $v'_i, v'_j$  (i.e.  $(v'_i - v'_j) \cdot \omega > 0$ ) through the relations

$$\begin{cases} v'_i = v_i - \omega[\omega \cdot (v_i - v_j)] \\ v'_j = v_j + \omega[\omega \cdot (v_i - v_j)] \end{cases} . \quad (1.3)$$

We recall that  $\Phi_N^t$  is a.e. well defined with respect to the Lebesgue measure [1, 26, 6].

For  $j = 1, 2, \dots, N$ , we denote by  $f_{0,j}^N$  and  $f_j^N(t)$  the  $j$ -particle marginals of  $W_0^N$  and  $W^N(t)$  respectively (e.g.  $f_j^N(t) = \int W^N(t) dz_{j+1} \cdots dz_N$ ). The main quantity of interest is then

$$f_1^{N, \Gamma_n}(z_1, t) = \int dz_2 \cdots dz_N \chi_{\Gamma_n} W^N(Z_N, t) \quad (1.4)$$

where  $\chi_{\Gamma_n}$  is the characteristic function of the event: *Particle 1 has a backward cluster of cardinality  $n$  with structure  $\Gamma_n$* . Eq. (1.4) is the restriction of the marginal  $f_1^N$  to trajectories with given cluster structure, hence  $f_1^N = \sum_n f_1^{N, n}$  where

$$f_1^{N, n} = \sum_{\Gamma_n} f_1^{N, \Gamma_n} . \quad (1.5)$$

The average cluster size at time  $t$  is

$$S^N(t) = \mathbb{E}^N(|BC(1)|) = \sum_{k=0}^{N-1} k \mathbb{P}^N(|BC(1)| = k) \quad (1.6)$$

where

$$\mathbb{P}^N(|BC(1)| = k) = \sum_{\Gamma_k} \int dz_1 f_1^{N, \Gamma_k}(z_1, t) . \quad (1.7)$$

We shall look for estimates of these quantities, uniformly in the Boltzmann-Grad scaling

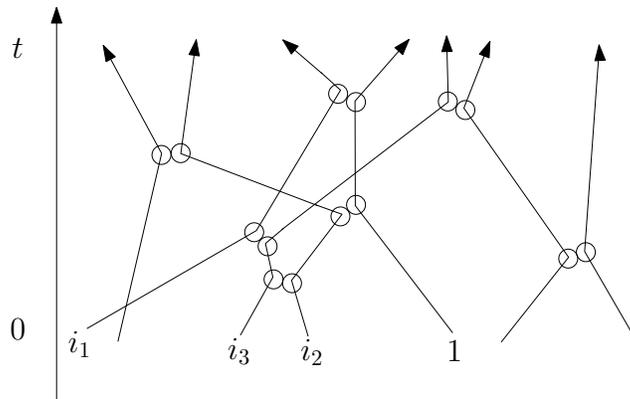
$$N \rightarrow \infty , \quad \varepsilon \rightarrow 0$$

where

$$\varepsilon^2 N = 1 . \quad (1.8)$$

Hence  $N$  is the only relevant parameter: from now on,  $\varepsilon$  is determined by the relation (1.8).

We conclude this section by mentioning still a different definition of cluster which has been studied considerably. Fixed a time  $t > 0$ , one can partition the entire system of particles into the maximal disjoint union of non-interacting (in  $[0, t]$ ) groups. Such groups are ‘dynamical clusters’ (called in [17] *Bogolyubov clusters*), generally bigger than the backward clusters of the particles composing them. Indeed in the backward cluster, the trajectory of each particle is specified only in a subinterval of  $(0, t)$ , see e.g. Figure 1; while the dynamical cluster “completes” the future history of particles  $i_1, i_2, \dots$ , together with the complete history (in  $[0, t]$ ) of the particles with whom they collide, and so on:



This leads to a *symmetrized* notion of cluster which does not depend on the direction of time [17]. Theoretical investigation of dynamical clusters has been performed in [23, 24, 8, 17, 18]. They have an interesting geometric property as they give rise to “percolation”

in finite time (close to the mean free time in the Boltzmann-Grad limit). That is, a giant, macroscopic cluster (of size  $O(N)$ ) emerges abruptly, so that after some critical time it is impossible to obtain an estimate of the mean size uniformly in  $N$ .

## 2 Main results

Let the initial probability measure  $W_0^N$  on the  $N$ -particle hard sphere system be given by the canonical Gibbs measure at temperature  $\beta^{-1} > 0$ :

$$W_{eq}^N(Z_N) := \frac{1}{\mathcal{Z}_N} \prod_{i=1}^N e^{-\frac{\beta}{2}v_i^2}, \quad (2.1)$$

where  $\mathcal{Z}_N$  is the normalization constant. Remind that this is a probability measure on the phase space (1.2), which takes into account the exclusion condition  $|x_i - x_j| > \varepsilon$ ,  $i \neq j$ , with  $\varepsilon$  given by (1.8). Moreover, the measure is time invariant for the hard-sphere flow.

Let  $f_{1,eq}^{N,\Gamma_n}$ ,  $f_{1,eq}^{N,n}$ ,  $S_{eq}^N$ ,  $\mathbb{P}_{eq}^N$  be given as in (1.4)-(1.7) for the equilibrium measure  $W_{eq}^N$ .

**Theorem 2.1.** *Given  $t > 0$ , there exist an integer  $k_0$  and a positive constant  $C$  such that the cardinality of backward clusters at time  $t$  satisfies, for  $k > k_0$ , the following inequality:*

$$\mathbb{P}_{eq}^N(|BC(1)| = k) \leq Ct e^{-\frac{1}{4}k^{\frac{1}{Ct}}}. \quad (2.2)$$

*In particular, the average cardinality  $S_{eq}^N(t)$  is bounded uniformly in  $N$  in any bounded interval of time.*

The integer  $k_0$  deteriorates for  $t/\sqrt{\beta}$  large, as expected. Moreover, the bound implies superexponential growth  $S_{eq}^N(t) = O(e^{C't \log t})$ ,  $C' > 0$  for  $t$  large, with  $C' \sim 1/\sqrt{\beta}$  for  $\beta$  small. This is compatible with the results of [2].

The same estimate holds true out of equilibrium, if one assumes strong uniform bounds on the marginals.

**Corollary 2.2.** *Let  $W^N(t)$  have marginals  $(f_j^N(t))_{j=1}^N$  obeying*

$$f_j^N(t) \prod_{i=1}^j e^{\frac{\beta}{2}v_i^2} \leq A^j, \quad t \in [0, T] \quad (2.3)$$

*for some  $A, \beta, T > 0$ . Then the cardinality of backward clusters at time  $t \in [0, T]$  satisfies Eq. (2.2).*

The proof of the corollary is exactly the same as the proof of the theorem, because only the bound (2.3) is used as property of the equilibrium marginals. As a consequence Eq. (2.2) is proven under the assumptions of [15], for times short enough (in fact as proved by Lanford, (2.3) holds true uniformly in the Boltzmann-Grad scaling).

Our results, combined with the results on the Boltzmann equation obtained in [2], suggest that the average growth of clusters is indeed exponential in time, at least for measures on which we have a very good control.

## 2.1 A heuristic bound

The probability that particle 1 has a backward cluster of cardinality  $k$  at time  $t$  can be estimated as follows. Suppose that all the particles have velocity of order 1. Some particle  $i_1$  has to lie in the collision cylinder spanned by 1 in  $(0, t)$ , which corresponds to a region of volume  $C(N-1)\varepsilon^2 t$  in the  $N$ -particle phase space, where  $C > 0$  is a geometrical constant. Similarly, the condition of existence of a second particle  $i_2$  restricts to a volume of order  $2C(N-1)(N-2)\varepsilon^4 t^2$  (because of the two possibilities:  $i_2$  can be “generated” by particle 1 or by particle  $i_1$ ). Iterating and using (1.8) we find that

$$\mathbb{P}^N(|BC(1)| = k) \leq \frac{(Ct)^k k!}{k!}, \quad (2.4)$$

where the  $k!$  at denominator arises from the time ordering which we have to take into account.

Eq. (2.4) is a rough bound, plausible for short times only. In fact the argument reminds Lanford’s proof of the local validity of the Boltzmann equation [15] (see also [13, 25, 6, 9, 19, 20, 7, 3, 10]). The estimate is too pessimistic, because it ignores that the particles not belonging to  $BC(1)$  do *not* interact with it, which produces exponential damping.

A simple way to provide an improved, formal estimate is the following. Fix  $\Gamma_k$  and focus on  $\int f_1^{N, \Gamma_k}(t)$ , the probability that particle 1 has a backward cluster of cardinality  $k$  with structure  $\Gamma_k$ . We partition the interval  $(0, t)$  into  $M$  disjoint small time intervals of length  $\delta = t/M$ . Then

$$\int f_1^{N, \Gamma_k} \approx \sum_{\substack{m_1, \dots, m_k \\ m_s=1, \dots, M \\ M \geq m_1 > m_2, \dots, m_k \geq 1}} \int f_1^{N, \Gamma_k} \chi_{m_1, \dots, m_k} \quad (2.5)$$

where  $\chi_{m_1, \dots, m_k}$  is the indicator of the event: *the  $k$  collisions of the backward cluster (recollisions excluded) take place in the time intervals  $((m_s - 1)\delta, m_s\delta)$ ,  $s = 1, \dots, k$* . Eq. (2.5) is not exact because we are assuming that in each time interval only one new particle

appears, an error which we neglect in view of the limit  $\delta \rightarrow 0$ . As before, the probability of the collisions in the small time intervals is approximately  $N\varepsilon^2\delta = \delta$ , but now we take into account the probability of the complement set  $1 - \delta$  (no collision generating new particles takes place in the other intervals). Thus the first collision of particle 1 in  $((m_1 - 1)\delta, m_1\delta)$  yields a contribution  $\delta(1 - \delta)^{M-m_1}$ , (taking into account that in the time interval  $(m_1\delta, t)$  particle 1 did not collide). The second collision of the tree yields  $\delta^2(1 - \delta)^{M-m_1}(1 - \delta)^{2(m_1-m_2)}(1 - \delta)^{-2}$ , and so on. In conclusion

$$\begin{aligned} \int f_1^{N, \Gamma_k} &\approx \sum_{\substack{m_1, \dots, m_k \\ m_s=1, \dots, M \\ M \geq m_1 > m_2, \dots, m_k \geq 1}} \frac{\delta^k}{(1 - \delta)^{\frac{k(k+3)}{2}}} (1 - \delta)^{(M-m_1)} (1 - \delta)^{2(m_1-m_2)} \dots (1 - \delta)^{(k+1)m_k} \\ &\approx \int_0^t dt_1 \dots \int_0^{t_{k-1}} dt_k e^{-(t-t_1)} e^{-2(t_1-t_2)} \dots e^{-k(t_{k-1}-t_k)} e^{-(k+1)t_k} = e^{-t} \frac{(1 - e^{-t})^k}{k!} \end{aligned}$$

as  $\delta \rightarrow 0$ . Indeed if  $t_i = m_i\delta$ :

$$(1 - \delta)^{(i+1)(m_i-m_{i+1})} = \left(1 - \frac{t}{M}\right)^{(i+1)(t_i-t_{i+1})\frac{M}{t}} \approx e^{-(i+1)(t_i-t_{i+1})}.$$

The reader might recognize the Riemann approximation of the term with structure  $\Gamma_k$  in the classical Wild sum (see e.g. [2], Section 3). Summing over all the trees (see (1.7)), we get

$$\mathbb{P}^N(|BC(1)| = k) \approx e^{-t}(1 - e^{-t})^k,$$

and the average size  $S^N(t) \approx e^t - 1$  is bounded for all positive times.

In essence, the above computation is equivalent to replacing the (difficult) computation of  $f^{N, \Gamma_n}(t)$ , with the computation of the ‘limiting quantity’ as given by a nice solution to the Boltzmann equation. Such a quantity is provided by the Wild sums which can be estimated in the case of homogeneous solutions. This has been done in fact in [2], and compared with molecular dynamics simulations, to argue that  $S^N(t)$  should increase exponentially in time:

$$(e^{ct} - 1) \leq S^N(t) \leq (e^{Ct} - 1)$$

for  $t$  large, for some  $c, C > 0$ .

### 3 Proof of Theorem 2.1

The proof is organized in two parts. In Section 3.1 we introduce a formula expressing integrals over paths of a given cluster, and give a first a priori bound on (1.5). This is

inspired by previous works on the Boltzmann-Grad limit. In Section 3.2 we prove (2.2), by controlling the dynamical representation on small, properly chosen time intervals obtained by partitioning  $(0, t)$ .

Throughout the proof,  $\chi_E$  will indicate the characteristic function of the set  $E$ .

### 3.1 Integrals over clusters

We start by introducing a notation for the trajectory of a backward cluster. For future convenience, we shall look at clusters on a fixed time interval  $[t^*, t]$  where  $0 \leq t^* < t$ . We still denote by  $BC(1)$  the backward cluster of 1, only in this subsection restricted to  $[t^*, t]$ . According to a terminology introduced in [20], the trajectory of such a cluster is called *interacting backwards flow* (IBF). We denote it by  $Z^{IBF}(s)$ ,  $s \in [t^*, t]$ . Note that there is no label specifying the number of particles. This number depends indeed on the time, as explained by the following construction.

Given  $\Gamma_k$ , we fix a collection of variables  $z_1, T_k, \Omega_k, V_{1,k}$ :

$$\begin{aligned} z_1 &\in \mathbb{T}^3 \times \mathbb{R}^3, \\ T_k &= (t_1, \dots, t_k) \in \mathbb{R}^k, \\ \Omega_k &= (\omega_1, \dots, \omega_k) \in \mathbb{S}^{2k}, \\ V_{1,k} &= (v_2, \dots, v_{1+k}) \in \mathbb{R}^{3k} \end{aligned}$$

where the times are constrained to be ordered as

$$t \equiv t_0 > t_1 > t_2 > \dots > t_k > t_{k+1} \equiv t^*,$$

and  $\Omega_k$  has to satisfy a further constraint that will be specified soon. If  $s \in (t_{r+1}, t_r)$ , then the IBF contains exactly  $1 + r$  particles:

$$Z^{IBF}(s) = (z_1^{IBF}(s), \dots, z_{1+r}^{IBF}(s)) \in \mathcal{M}_{1+r} \quad \text{for } s \in (t_{r+1}, t_r),$$

with

$$z_i^{IBF}(s) = (\xi_i(s), \eta_i(s)),$$

respectively the position and the velocity of particle  $i$  in the flow. The trajectory  $Z^{IBF}(s)$  is constructed starting from the configuration  $z_1$  at time  $t > 0$ , and going back in time. A new particle appears (is “created”) at time  $t_r$  in a collision state with a previous particle  $k_r \in \{1, \dots, r\}$ , specified by  $\Gamma_k$ . More precisely, in the time interval  $(t_r, t_{r-1})$  particles  $1, \dots, r$  flow according to the interacting dynamics of  $r$  hard spheres. This defines  $Z_r^{IBF}(s)$  starting from  $Z_r^{IBF}(t_{r-1})$ . At time  $t_r$  the particle  $1 + r$  is created by particle  $k_r$  in the position  $\xi_{1+r}(t_r) = \xi_{k_r}(t_r) + \omega_r \varepsilon$  and with velocity  $v_{1+r}$ . This defines

$Z^{IBF}(t_r) = (z_1^{IBF}(t_r), \dots, z_{1+r}^{IBF}(t_r))$ . A constraint on  $\omega_r$  is imposed ensuring that two hard spheres cannot be at distance smaller than  $\varepsilon$ . Next, the evolution in  $(t_{r+1}, t_r)$  is constructed applying to this configuration the dynamics of  $1 + r$  spheres. Since, by construction,  $\omega_r \cdot (v_{1+r} - \eta_{k_r}(t_r^+)) \geq 0$ , the pair is post-collisional. Then the presence of the interaction in the hard-sphere flow forces the pair to perform a (backwards) instantaneous collision. Proceeding inductively, the IBF is constructed for all times  $s \in [t^*, t]$ .

Observe that, to denote the explicit dependence on the whole set of variables, we should write

$$Z^{IBF}(s) = Z^{IBF}(s; \Gamma_k, z_1, T_k, \Omega_k, V_{1,k}), \quad s \in [t^*, t]. \quad (3.1)$$

We shall however use always the abbreviated notation.

Let  $\mathcal{A}(\Gamma_k) \subset \mathcal{M}_N$  be the set of variables  $Z_N$  such that the trajectory  $\Phi_N^{-(t-s)}(Z_N)$ ,  $s \in [t^*, t]$ , satisfies the following constraints:

- (i) the backward cluster of 1 in  $[t^*, t]$  is given by  $BC(1) = \{2, \dots, 1+k\}$ ;
- (ii) the structure of  $BC(1)$  is given by  $\Gamma_k$
- (iii) the backward cluster has  $n'$  creations in  $[t', t]$  and  $k - n'$  creations in  $[t^*, t')$ , for some intermediate time  $t' \in [t^*, t]$ .

We introduce a map  $\mathcal{J}$  on  $\mathcal{A}(\Gamma_k)$  by

$$\mathcal{J}(Z_N) = (z_1, T_k, \Omega_k, V_{1,k}, Z_{1+k, N-k-1}(t^*)) \quad (3.2)$$

where  $(z_1, T_k, \Omega_k, V_{1,k})$  is the set of variables such that (3.1) provides the trajectory of  $\{1\} \cup BC(1)$ , and  $Z_{1+k, N-k-1}(t^*) = z_{k+2}(t^*), \dots, z_N(t^*)$  is the configuration of the remaining particles at time  $t^*$ . The map  $\mathcal{J}$  is invertible on  $\mathcal{A}(\Gamma_k)$  and its Jacobian determinant has absolute value

$$\varepsilon^{2k} \prod_{i=1}^k \omega_i \cdot (v_{1+i} - \eta_{k_i}(t_i^+))$$

(positive by construction). To construct  $\mathcal{J}^{-1}$ , one determines first the IBF (3.1) using the variables  $z_1, T_k, \Omega_k, V_{1,k}$ . Secondly one adds the variables  $Z_{1+k, N-k-1}$ , and consider  $(Z^{IBF}(t^*), Z_{1+k, N-k-1})$  as initial condition for the flow  $\Phi_N^s$ ,  $s \in [0, t - t^*]$ . By construction, the variables external to the backward cluster do not interfere with it. Therefore by uniqueness of the hard sphere dynamics,  $\Phi_N^t(Z^{IBF}(t^*), Z_{1+k, N-k-1})$  is determined.

Let

$$B_i = (\omega_i \cdot (v_{1+i} - \eta_{k_i}(t_i^+)))_+ \chi_{\{|\xi_{1+i}(t_i) - \xi_k(t_i)| > \varepsilon \ \forall k \neq k_i\}}.$$

Notice that the constraint ensures non-overlap of hard spheres in the IBF (at the creation

times). Using the Liouville equation and (3.2), we have that

$$\begin{aligned} & \int_{\mathcal{A}(\Gamma_k)} dz_2 \cdots dz_N W^N(Z_N, t) \\ &= \varepsilon^{2k} \int d\Lambda_{\Gamma_k} \prod_{i=1}^k B_i W^N(Z_{1+k}^{IBF}(t^*), Z_{1+k, N-k-1}, t^*) \end{aligned} \quad (3.3)$$

where

$$d\Lambda_{\Gamma_k} = dT_k d\Omega_k dV_{1,k} dZ_{1+k, N-k-1} \chi_{\{t > t_1 > t_2 \cdots > t_k > t^*\}} \chi_{\mathcal{J}(\mathcal{A}(\Gamma_k))}$$

Notice that  $\mathcal{J}(\mathcal{A}(\Gamma_k))$  is a rather intricate subset of the full domain of integration. It depends on all the variables and in particular it imposes restrictions on particles  $1+i$  concerning their behaviour in  $(t_i, t)$ .

Ignoring the restriction to  $\mathcal{J}(\mathcal{A}(\Gamma_k))$  and using the definition of marginal, we obtain a first estimate:

$$\int_{\mathcal{A}(\Gamma_k)} dz_2 \cdots dz_N W^N(Z_N, t) \leq \varepsilon^{2k} \int d\Lambda_k \chi_{\{t_{n'} > t' > t_{n'+1}\}} \prod_{i=1}^k B_i f_{1+k}^N(Z_{1+k}^{IBF}(t^*), t^*), \quad (3.4)$$

where

$$d\Lambda_k = dT_k d\Omega_k dV_{1,k} \chi_{\{t > t_1 > t_2 \cdots > t_k > t^*\}}$$

and  $\chi_{\{t_{n'} > t' > t_{n'+1}\}}$  comes from condition (iii) above.

Moreover, the following uniform bound is well known. It is essentially equivalent to Lanford's a priori bound providing the short time validity result [15].

**Lemma 3.1.** *Suppose that there exist  $A, \beta > 0$  such that*

$$f_j^N(Z_j, t^*) e^{+\frac{\beta}{2} \sum_{i=1}^j v_i^2} \leq A^j \quad (3.5)$$

for all  $j = 1, \dots, N$  and  $Z_j \in \mathcal{M}_j$ . Then there exists  $C_1 = C_1(A, \beta) > 0$  such that, for all  $k \geq 1$  and  $t' \in [t^*, t]$ ,

$$\sum_{\Gamma_k} \int d\Lambda_k \chi_{\{t_{n'} > t' > t_{n'+1}\}} \prod_{i=1}^k B_i f_{1+k}^N(Z_{1+k}^{IBF}(t^*), t^*) \leq e A C_1^k (t-t')^{n'} (t-t')^{k-n'} e^{-\frac{\beta}{4} v_1^2}. \quad (3.6)$$

The proof of the lemma is recalled in Appendix.

### 3.2 Estimate of $|BC(1)|$

Given an arbitrary but fixed  $t > 0$ , we write  $t = m\tau$  where  $\tau > 0$ , sufficiently small, will be chosen later on. We partition the interval  $[0, t]$  into  $m$  intervals  $[0, \tau)$ ,  $[\tau, 2\tau)$ ,  $\dots$ ,  $[(m-1)\tau, m\tau = t]$ . The intervals are indexed by  $i = 1, 2, \dots, m$  respectively. For any integer  $k > 0$ , we assign to the  $i$ -th interval the number

$$\kappa_i = \frac{k^{\frac{m-i+1}{m}}}{2},$$

to be used as a cutoff on the local growth of the cluster. The sequence is decreasing

$$\kappa_1 = \frac{k}{2}, \quad \kappa_2 = \frac{k^{\frac{m-1}{m}}}{2}, \quad \dots, \quad \kappa_m = \frac{k^{\frac{1}{m}}}{2}$$

and

$$\frac{\kappa_i}{k} \rightarrow 0 \quad (i \neq 1), \quad \frac{\kappa_{i+1}}{\kappa_i} = k^{-\frac{1}{m}} \rightarrow 0$$

as  $k$  diverges.

By (1.4)-(1.5),

$$\begin{aligned} f_{1,eq}^{N,k}(z_1, t) &= \sum_{\Gamma_k} \int dz_2 \cdots dz_N \chi_{\Gamma_k} W_{eq}^N(Z_N) \\ &= (N-1) \cdots (N-k) \sum_{\Gamma_k} \int dz_2 \cdots dz_N \chi_{\Gamma_k}^{ord} W_{eq}^N(Z_N) \\ &= (N-1) \cdots (N-k) \sum_{\substack{n_1 \cdots n_m: \\ \sum_{i=1}^m n_i = k}} \sum_{\Gamma_k} \int dz_2 \cdots dz_N \chi_{\Gamma_k}^{ord} \chi_{\{n_1, \dots, n_m\}} W_{eq}^N(Z_N). \end{aligned} \tag{3.7}$$

Recall that  $\chi_{\Gamma_k}$  is the characteristic function of particle 1 having a backward cluster of cardinality  $k$  with structure  $\Gamma_k$ . Similarly  $\chi_{\Gamma_k}^{ord}$  is the characteristic function of particle 1 having the backward cluster  $BC(1) = \{2, \dots, k+1\}$ , with structure  $\Gamma_k$ . The second identity in (3.7) is due to the symmetry of the measure. Finally by definition, the characteristic function of the set  $\{n_1, \dots, n_m\}$  constrains the number of creations in the backward cluster in the interval  $[(i-1)\tau, i\tau)$  to be exactly  $n_i$ .

We insert now the partition of unity

$$1 = \sum_{s=1}^m \prod_{i=s+1}^m \chi_{\{n_i \leq \kappa_i\}} \chi_{\{n_s > \kappa_s\}} + \prod_{i=1}^m \chi_{\{n_i \leq \kappa_i\}}.$$

Note that  $\prod_{i=1}^m \chi_{\{n_i \leq \kappa_i\}} = 0$  for  $k$  large enough since

$$\sum_{i=1}^m n_i \leq \sum_{i=1}^m \kappa_i \leq \frac{k + (m-1)k^{\frac{m-1}{m}}}{2} \leq \frac{2}{3}k$$

for  $k$  large (depending on  $m$ ), so that condition  $\sum n_i = k$  implies that there exists at least an interval for which  $n_s > \kappa_s$ . Therefore

$$\begin{aligned} f_{1,eq}^{N,k}(z_1, t) &= (N-1) \cdots (N-k) \sum_{s=1}^m \\ &\times \sum_{\substack{n_1 \cdots n_m: \\ \sum_{i=1}^m n_i = k}} \sum_{\Gamma_k} \int dz_2 \cdots dz_N W_{eq}^N(Z_N) \chi_{\{n_1, \dots, n_m\}} \left( \prod_{i=s+1}^m \chi_{\{n_i \leq \kappa_i\}} \right) \chi_{\{n_s > \kappa_s\}} \chi_{\Gamma_k}^{ord}. \end{aligned}$$

We set  $\bar{n}_s = \sum_{i=s+1}^m n_i$ ,  $\bar{\kappa}_s = \sum_{i=s+1}^m \kappa_i$  and  $\chi_{\{\bar{n}_s, n_s\}}^s$  the indicator function of having  $\bar{n}_s$  creations in the time interval  $[s\tau, t]$  and  $n_s$  creations in the interval  $[(s-1)\tau, s\tau)$ . Note then that the last line in the previous formula is bounded above by

$$\begin{aligned} &\sum_{\bar{n}_s \leq \bar{\kappa}_s} \sum_{n_s > \kappa_s} \sum_{\Gamma_k} \int W_{eq}^N \chi_{\{\bar{n}_s, n_s\}}^s \chi_{\Gamma_k}^{ord} \\ &\leq \frac{1}{(N-1-\bar{n}_s-n_s) \cdots (N-k)} \sum_{\bar{n}_s \leq \bar{\kappa}_s} \sum_{n_s > \kappa_s} \sum_{\Gamma_{\bar{n}_s+n_s}} \int W_{eq}^N \chi_{\{\bar{n}_s, n_s\}}^s \chi_{\Gamma_{\bar{n}_s+n_s}}^{ord,s}, \end{aligned}$$

where in the last step we eliminated the sum over all trees in  $[0, (s-1)\tau)$ , and  $\chi_{\Gamma_{\bar{n}_s+n_s}}^{ord,s}$  is the characteristic function of particle 1 having the backward cluster  $\{2, \dots, \bar{n}_s + n_s + 1\}$  with structure  $\Gamma_{\bar{n}_s+n_s}$  in  $[(s-1)\tau, t]$ . In this way we have removed any constraint on the trajectory in the time interval  $[0, (s-1)\tau)$ , thus

$$\begin{aligned} f_{1,eq}^{N,k}(z_1, t) &\leq \sum_{s=1}^m \sum_{\bar{n}_s \leq \bar{\kappa}_s} \sum_{n_s > \kappa_s} (N-1) \cdots (N-\bar{n}_s-n_s) \\ &\times \sum_{\Gamma_{\bar{n}_s+n_s}} \int dz_2 \cdots dz_N W_{eq}^N(Z_N) \chi_{\{\bar{n}_s, n_s\}}^s \chi_{\Gamma_{\bar{n}_s+n_s}}^{ord,s}. \end{aligned}$$

Applying now (3.4) (with  $k \rightarrow \bar{n}_s + n_s$ ,  $t^* = (s-1)\tau$ ,  $t' = s\tau$  and  $n' = \bar{n}_s$ ), we arrive to

$$\begin{aligned} f_{1,eq}^{N,k}(z_1, t) &\leq \sum_{s=1}^m \sum_{r_1 \leq \bar{\kappa}_s} \sum_{r_2 > \kappa_s} \sum_{\Gamma_{r_1+r_2}} \varepsilon^{2(r_1+r_2)} (N-1) \cdots (N-r_1-r_2) \\ &\times \int d\Lambda_{r_1+r_2} \chi_{\{t_{r_1} > s\tau > t_{r_1+1}\}} \prod_{i=1}^{r_1+r_2} B_i f_{1+r_1+r_2,eq}^N(Z_{1+r_1+r_2}^{IBF}((s-1)\tau)). \end{aligned}$$

Since  $\varepsilon^{2(r_1+r_2)}(N-1)\cdots(N-r_1-r_2) \leq 1$ , by Lemma 3.1 we conclude that

$$f_{1,eq}^{N,k}(z_1, t) \leq \sum_{s=1}^m \sum_{r_1 \leq \bar{\kappa}_s} \sum_{r_2 > \kappa_s} eA C_1^{r_1+r_2} t^{r_1} \tau^{r_2} e^{-\frac{\beta}{4}v_1^2}.$$

We therefore choose  $m = \lceil 2C_1 t \rceil$ , hence  $\tau \leq \frac{1}{2C_1}$  which implies

$$f_{1,eq}^{N,k}(z_1, t) \leq \sum_{s=1}^m (C_2 t)^{\bar{\kappa}_s} \left(\frac{1}{2}\right)^{\kappa_s} e^{-\frac{\beta}{4}v_1^2}$$

for some large enough  $C_2 > 0$ . Since  $\bar{\kappa}_s \leq m \kappa_{s+1} = m k^{-\frac{1}{m}} \kappa_s$ , it follows that

$$f_{1,eq}^{N,k}(z_1, t) \leq \sum_{s=1}^m \left[ \frac{1}{2} (C_2 t)^{m k^{-\frac{1}{m}}} \right]^{\kappa_s} e^{-\frac{\beta}{4}v_1^2}.$$

The term in square brackets can be made smaller than  $1/\sqrt{e}$  for  $k$  large enough, hence (2.2) is obtained after integrating in  $z_1$ .  $\square$

## Appendix: Proof of Lemma 3.1

The conservation of energy at collisions implies

$$\sum_{i=1}^{1+k} (\eta_i(0))^2 = \sum_{i=1}^{1+k} v_i^2.$$

In particular  $\sum_{k_i=1}^i (\eta_{k_i}(t_i^+))^2 \leq \sum_{i=1}^{1+k} v_i^2$ . It follows that

$$\sum_{\Gamma_k} \prod_{i=1}^k B_i \leq \prod_{i=1}^k \left[ (1+k)|v_{1+i}| + (1+k)^{\frac{1}{2}} \left( \sum_{l=1}^{1+k} v_l^2 \right)^{\frac{1}{2}} \right].$$

Moreover

$$\left( \sum_{l=1}^{1+k} v_l^2 \right)^{\frac{1}{2}} e^{-\frac{\beta}{4k} \sum_{i=1}^{1+k} v_i^2} \leq \sqrt{\frac{2k}{e\beta}}.$$

Using the assumption (3.5) in the l.h.s. of (3.6), the estimates above imply that we can bound it by

$$e^{-(\beta/4)v_1^2} A \int dT_k d\Omega_k dV_{1,k} \chi_{\{t_{n'} > t' > t_{n'+1}\}} \prod_{i=1}^k e^{-\frac{\beta}{4}v_{1+i}^2} \left( (1+k)|v_{1+i}| + \frac{\sqrt{2k(1+k)}}{\sqrt{e\beta}} \right). \quad (\text{A.1})$$

The integral on the velocities factorizes so that

$$(A.1) \leq e^{-(\beta/4)v_1^2} A C_\beta^k \frac{(t-t')^{n'} (t'-t^*)^{k-n'}}{n'!(k-n')!} (1+k)^k$$

for a suitable constant  $C_\beta > 0$  (explicitly computable in terms of gaussian integrals). Since

$$\frac{(1+k)^k}{n'!(k-n')!} \leq 2^k \frac{(1+k)^k}{k!} \leq 2^k \frac{(1+k)^{1+k}}{(1+k)!} \leq 2^k e^{1+k},$$

we obtain (3.6).

**Acknowledgments.** We thank the hospitality of the HIM during the Bonn Junior Trimester Program *Kinetic Theory* in 2019, where this work was started.

## References

- [1] R.K. Alexander. The infinite hard sphere system. *Thesis*, Dep. of Mathematics, University of California at Berkeley (1975).
- [2] K. Aoki, M. Pulvirenti, S. Simonella and T. Tsuji. Backward clusters, hierarchy and wild sums for a hard sphere system in a low-density regime. *Math. Mod. Meth. Appl. Sci.* **25**(5), 995-1010 (2015).
- [3] T. Bodineau, I. Gallagher, L. Saint-Raymond and S. Simonella. One-sided convergence in the Boltzmann-Grad limit. *Ann. Fac. Sci. Toulouse Math. Ser. 6* **27**(5), 985-1022 (2018).
- [4] T. Bodineau, I. Gallagher, L. Saint-Raymond and S. Simonella. Fluctuation theory in the Boltzmann-Grad limit. *J. Stat. Phys.* **180**, 873-895 (2020).
- [5] D. Burago, S. Ferleger and A. Kononenko. Uniform estimates on the number of collisions in semi- dispersing billiards. *Ann. of Math.* **2** **147**(3), 695-708 (1998).
- [6] C. Cercignani, R. Illner and M. Pulvirenti. The mathematical theory of dilute gases. Springer-Verlag, New York (1994).
- [7] R. Denlinger. The propagation of chaos for a rarefied gas of hard spheres in the whole space. *Arch. Rat. Mech. Anal.* **229**, 885-952 (2018).

- [8] A. Gabriellov, V. Keilis-Borok, Ya. Sinai and I. Zaliapin. Statistical Properties of the Cluster Dynamics of the Systems of Statistical Mechanics. In: *Boltzmann's Legacy*, ESI Lectures in Mathematics and Physics, EMS Publishing House, 203–216 (2008).
- [9] I. Gallagher, L. Saint Raymond and B. Texier. From Newton to Boltzmann: hard spheres and short-range potentials. *Zürich Adv. Lect. in Math. Ser.* **18**, EMS (2014).
- [10] V.I. Gerasimenko and I.V. Gapyak. The Boltzmann-Grad asymptotic behavior of collisional dynamics: a brief survey. *Rev. Math. Phys.* **33** (2021).
- [11] H. Grad. On the kinetic theory of rarefied gases. *Comm. Pure App. Math.* **2**(4), 331–407 (1949).
- [12] H. Grad. Principles of the kinetic theory of gases. In *Handbuch der Physik* **3**, 205-294, Springer-Verlag (1958).
- [13] R. Illner and M. Pulvirenti. Global Validity of the Boltzmann equation for a Two- and Three-Dimensional Rare Gas in Vacuum: Erratum and Improved Result. *Comm. Math. Phys.* **121**, 143–146 (1989).
- [14] F. King. BBGKY hierarchy for positive potentials. *Ph.D. Thesis*, Department of Mathematics, Univ. California, Berkeley (1975).
- [15] O.E. Lanford. Time evolution of large classical systems. *Lect. Notes Phys.* **38**, 1–111 (1975).
- [16] T.J. Murphy and E.G.D. Cohen. On the Sequences of Collisions Among Hard Spheres in Infinite Space. In: Szász D. (eds) *Hard Ball Systems and the Lorentz Gas. Enc. of Math. Sci. (Math. Phys. II)* **101**, Springer, Berlin, Heidelberg (2000).
- [17] R. I. A. Patterson, S. Simonella and W. Wagner. Kinetic Theory of Cluster Dynamics. *Phys D: Nonlin. Phen.* **335**, 26–32 (2016).
- [18] R. I. A. Patterson, S. Simonella and W. Wagner. A kinetic equation for the distribution of interaction clusters in rarefied gases. *J. Stat. Phys.*, **169**(1), 126–167 (2017).

- [19] M. Pulvirenti, C. Saffirio and S. Simonella. On the validity of the Boltzmann equation for short-range potentials. *Rev. Math. Phys.* **26**, 1–64 (2014).
- [20] M. Pulvirenti and S. Simonella. The Boltzmann-Grad limit of a hard sphere system: analysis of the correlation error. *Invent. Math.* **207**(3), 1135-1237, (2017).
- [21] M. Pulvirenti and S. Simonella. A kinetic model for epidemic spread. *M&MOCS* **8**(3), 249-260 (2020).
- [22] D. Serre. Hard spheres dynamics: weak *vs* strong collisions. *Arch. Rat. Mech. Anal.* **240**(1), 1-22 (2021).
- [23] Y. Sinai. Construction of dynamics in one-dimensional systems of statistical mechanics. *Theor. Math. Phys.* **11**(2), 487-494 (1972).
- [24] Y. Sinai. Construction of a cluster dynamic for the dynamical systems of statistical mechanics. *Moscow Univ. Math. Bull.* **29**(1) 124-129 (1974).
- [25] H. Spohn. Large-Scale Dynamics of Interacting Particles. Springer, Berlin (1991).
- [26] L.N. Vaserstein. On systems of particles with finite range and/or repulsive interactions. *Comm. Math. Phys.* **69**, 31-56 (1979).
- [27] E. Wild. On Boltzmann’s equation in the kinetic theory of gases. *Proc. Cambridge Philos. Soc.* **47**, 602-609 (1951).