Cluster expansion for a dilute hard sphere gas dynamics

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In [BGSRS20c], a cluster expansion method has been developed to study the fluctuations of the hard sphere dynamics around the Boltzmann equation. This method provides very precise controls on the exponential moments of the empirical measure from which the fluctuating Boltzmann equation and large deviation estimates have been deduced.

The cluster expansion in [BGSRS20c] was implemented at the level of the BBGKY hierarchy which is a standard tool to study the hard sphere gas dynamics [CIP94]. In this paper, we introduce a different approach to derive the cluster expansion directly from real trajectories of the particle system. This alternative approach allow us to recover the results obtained in [BGSRS20c] and it offers a fresh perspective on the study of the hard sphere dynamics as it bypasses the standard Duhamel series expansion.

I. INTRODUCTION

A gas dynamics can be modelled by a billiard made of hard spheres, moving according to the laws of classical mechanics. Initially the spheres are randomly distributed according to a probability measure which is then transported by the flow of the deterministic dynamics. For a dilute gas, it has been shown in the seminal work of Lanford [Lan75] that in the Boltzmann-Grad limit, the gas density converges towards the Boltzmann equation (at least for a short time). This work triggered a wave of developments [Spo12, CIP94, CGP97] including more recently quantitative convergence results and generalisations to the case of compactly supported potentials [GST14, PSS14, PS17]. In all these studies, the starting point is to consider evolution equations for the correlation functions which are finite dimensional projections of the probability distribution on all the particles. Concretely, the k-particle correlation function $F_k\big(t,(x_i,v_i)_{i\le k}\big)$ describes the distribution at time t of k particles with positions denoted by x_i and velocities by v_i. These correlation functions obey the well known BBGKY hierarchy which states that, due to collisions, the evolution of the density of k particles depends on the density of $k+1$ particles. As a consequence, the density of a typical particle does not follow an autonomous equation and a substantial amount of work is required to prove that the correlation functions factorise in the Boltzmann-Grad limit and that the evolution equations can be closed with only the first correlation function.

The equations of the BBGKY hierarchy are singular [Sim14, GST14] and it is more convenient mathematically to represent the particle density in terms of iterated Duhamel series which provides a practical tool to detect collisions responsible for memory and dynamical correlations. This series relates the density of a typical particle at time t to the initial random probability measure by applying intertwined transport and collision operators. Ultimately this representation is studied by interpreting these operators as integrals over pseudo-trajectories. As the goal of this paper is to bypass the iterated Duhamel representation, we will not explain this setting in more detail and refer to [CIP94] for an introduction to this method. Let us simply stress, that one possible disadvantage of the iterated Duhamel representation is that the microscopic dynamics is not used directly and the analysis is carried out by constructing pseudo-trajectories which do not correspond to physical trajectories. The link between BBGKY hierarchy and physical trajectories is indeed very indirect (see [Sim14]). Another feature of this hierarchical procedure is that the pseudo-trajectories are time-oriented, and followed backwards up to the initial time; which may appear to be at variance with the naive idea of a stochastic process.

In [BGSRS20c], the analysis of the correlation functions has been improved in order to control the fluctuations of the empirical measure and not only its mean. The key feature is the computation of the precise asymptotics for the exponential moment of the empirical measure. From this, several results can be derived, namely the fluctuating Boltzmann equation and the large deviations for the hard sphere dynamics. We refer to [BGSRS20a] (and references therein) for a survey on these results and their physical interpretation, including the relation with stochastic particle dynamics (Kac process).

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In this paper, we focus on the derivation of the asymptotics of the exponential moment and implement a different cluster expansion approach from the one developed in [BGSRS20c]. Cluster expansion has a long history originating in statistical mechanics, where it has been widely used to analyse Gibbs measures and the equilibrium behaviour of particle systems. Originally cluster expansion was designed to study gases in the low density regime and to establish thermodynamic relations in the spirit of the Virial expansion (see e.g. [Rue99]). This powerful method was then applied to more general contexts provided some relevant observables could be identified as weakly (or rarely) interacting. For example, for the Ising model in the phase transition regime, the relevant observables are no longer the spins, but the spin contours which form a dilute gas of contours at low temperature (see e.g. [FV17]). More recently, the theory was extended to an abstract framework covering continuous particle systems and polymers at low density [PU09]. In this paper, we apply the cluster expansion on the hard sphere dynamics and identify the relevant observables as the space/time clusters of particles interacting dynamically by collisions during a given time interval $[0,T]$. We show that for some time $T>0$, the interactions are sufficiently rare so that the cluster expansion can be implemented directly at the level of the particle trajectories, without relying on the standard Duhamel representation of the BBGKY hierachy. This new method provides results of the same nature than the one derived in [BGSRS20c]. In particular, we will show in Proposition III.3 that a correspondence between Theorem 6 of [BGSRS20c] and our new representation can be established in the Boltzmann-Grad limit. The cluster expansion method replaces the (iterated) BBGKY hierarchy by a refined combinatorial formula on (real) trajectories of the particle system. Compared to [BGSRS20c], this provides an alternative take on the Boltzmann-Grad limit, with twofold interest: (i) a more direct link with physical trajectories; (ii) a representation of observables in terms of a forward-in-time process, with randomness entering through the initial measure; see also [MT12] for an approach sharing analogies with ours. This representation can be easier to follow for some readers, although it involves more delicate combinatorics than the one discussed by Lanford to derive the Boltzmann equation. Indeed the cluster expansion is tailored on the exponential moments containing a larger amount of information on the correlations; from which the validity of the Boltzmann equation is obtained as a byproduct (see Section III B below).

A. The model

We consider a microscopic model of identical hard spheres of unit mass and of diameter ε. The motion of N such hard spheres is ruled by a system of ordinary differential equations, which are set in $(\mathbb{T}^d \times \mathbb{R}^d)^N$ where $\mathbb{T}^d = [0,1]^d$ is the unit d-dimensional periodic box with $d \geq 2$: writing $\mathbf{x}_i^\varepsilon \in \mathbb{T}^d$ for the position of the center of the particle labeled by i and $\mathbf{v}_i^\varepsilon \in \mathbb{R}^d$ for its velocity, one has

$$\frac{d\mathbf{x}_i^\varepsilon}{dt} = \mathbf{v}_i^\varepsilon, \quad \frac{d\mathbf{v}_i^\varepsilon}{dt} = 0 \quad \text{as long as } |\mathbf{x}_i^\varepsilon(t) - \mathbf{x}_j^\varepsilon(t)| > \varepsilon \quad \text{for } 1 \leq i \neq j \leq N, \tag{1}$$

with specular reflection at collisions, i.e. when $|\mathbf{x}_i^\varepsilon(t) - \mathbf{x}_j^\varepsilon(t)| = \varepsilon$

$$\begin{cases} (\mathbf{v}_i^\varepsilon)' := \mathbf{v}_i^\varepsilon - \big((\mathbf{v}_i^\varepsilon - \mathbf{v}_j^\varepsilon)\cdot\boldsymbol{\omega}\big)\boldsymbol{\omega} \\ (\mathbf{v}_j^\varepsilon)' := \mathbf{v}_j^\varepsilon + \big((\mathbf{v}_i^\varepsilon - \mathbf{v}_j^\varepsilon)\cdot\boldsymbol{\omega}\big)\boldsymbol{\omega} \end{cases} \tag{2}$$

where $\boldsymbol{\omega} = (\mathbf{x}_i^\varepsilon(t) - \mathbf{x}_j^\varepsilon(t))/\varepsilon$ is the unit vector pointing along the relative position at the collision time t. The collections of N positions and velocities are denoted respectively by $X_N := (x_1, \dots, x_N)$ in $\mathbb{T}^{dN}$ and $V_N := (v_1, \dots, v_N)$ in $\mathbb{R}^{dN}$, and we set $Z_N := (X_N, V_N)$, with $Z_N = (z_1, \dots, z_N)$, $z_i = (x_i, v_i)$. A set of N particles is characterized by a random variable $\mathbf{Z}_N^{\varepsilon 0} = (\mathbf{z}_1^{\varepsilon 0}, \dots, \mathbf{z}_N^{\varepsilon 0})$ specifying the time-zero configuration in the phase space

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

and an evolution

$$t \to \mathbf{Z}_N^\varepsilon(t) = \left(\mathbf{z}_1^\varepsilon(t), \dots, \mathbf{z}_N^\varepsilon(t)\right), \qquad t > 0$$

according to the deterministic flow (1)-(2) (well defined almost surely under the Lebesgue measure [Ale75]).

The dynamics is deterministic, but the initial data are chosen randomly according to the grand canonical formalism described below (see [Rue99] for details). The number of particles $\mathcal{N}$ is a random variable so that the initial measure is defined on the phase space

$$\mathcal{D}^\varepsilon := \bigcup_{N \geq 0} \mathcal{D}_N^\varepsilon$$

(notice that $\mathcal{D}_N^\varepsilon = \varnothing$ for N large due to the exclusion condition). Initially, the probability density of finding N particles with configuration Z_N is given by

$$\frac{1}{N!} M_N^\varepsilon(Z_N) := \frac{1}{\mathcal{Z}^\varepsilon} \frac{\mu_\varepsilon^N}{N!} \mathbf{1}_{\mathcal{D}_N^\varepsilon}(Z_N) \prod_{i=1}^N f^0(z_i), \tag{4}$$

where the distribution of a single particle f^0 is a Lipschitz continuous function on $\mathbb{T}^d \times \mathbb{R}^d$ satisfying the following bound for some constants $\beta, C_0 > 0$

$$\forall z \in \mathbb{T}^d \times \mathbb{R}^d, \quad f^0(z) \leq C_0 \mathcal{M}_\beta(v) \quad \text{with} \quad \mathcal{M}_\beta(v) := \frac{1}{(2\pi\beta)^{\frac{d}{2}}} \exp\left(-\beta \frac{|v|^2}{2}\right), \tag{5}$$

and the partition function is given by

$$\mathcal{Z}^\varepsilon := 1 + \sum_{N \geq 1} \frac{\mu_\varepsilon^N}{N!} \int_{(\mathbb{T}^d \times \mathbb{R}^d)^N} \mathbf{1}_{\mathcal{D}_N^\varepsilon}(Z_N) \prod_{i=1}^N f^0(z_i)\, dZ_N. \tag{6}$$

The probability of an event A with respect to the measure (4) will be denoted $\mathbb{P}_\varepsilon(A)$, and $\mathbb{E}_\varepsilon$ will be the expectation.

In the low density regime, referred to as the Boltzmann-Grad scaling, the density (average $\mathcal{N}$) is tuned by the parameter

$$\mu_\varepsilon := \varepsilon^{-(d-1)}, \tag{7}$$

ensuring that the mean free path between collisions is of order one [Gra49]. Definition (4) implies that

$$\lim_{\varepsilon \to 0} \mu_\varepsilon^{-1} \mathbb{E}_\varepsilon(\mathcal{N}) = 1.$$

As mentioned earlier in the introduction, the key result originally derived by Lanford [Lan75] is the convergence of the first correlation function to the solution of the Boltzmann equation with initial data f^0

$$\begin{cases} \partial_t f + v\cdot\nabla_x f = \displaystyle\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} \Big(f(t,x,w')f(t,x,v') - f(t,x,w)f(t,x,v)\Big)\Big((v-w)\cdot\omega\Big)_+ d\omega\, dw, \\ f(0,x,v) = f^0(x,v) \end{cases} \tag{8}$$

where the precollisional velocities (v',w') are defined by the scattering law

$$v' := v - \big((v-w)\cdot\omega\big)\,\omega, \qquad w' := w + \big((v-w)\cdot\omega\big)\,\omega. \tag{9}$$

This can be rephrased in terms of the convergence of the empirical density

$$\pi_t^\varepsilon := \frac{1}{\mu_\varepsilon}\sum_{i=1}^{\mathcal{N}} \delta_{\mathbf{z}_i^\varepsilon(t)} \tag{10}$$

which is the relevant observable to describe the time evolution of the hard-sphere model. More generally, we are interested in the whole path of particle trajectories during a given time interval $[0,T]$. Let $\mathbb{D}([0,T],\mathbb{T}^d\times\mathbb{R}^d)$ be the set of single particle trajectories $\mathbf{z}^\varepsilon([0,T])$, which are functions piecewise linear continuous in position and piecewise constant in velocity. Then the generalised empirical measure is defined by

$$\pi_{[0,T]}^\varepsilon := \frac{1}{\mu_\varepsilon}\sum_{i=1}^{\mathcal{N}} \delta_{\mathbf{z}_i^\varepsilon([0,T])}\,. \tag{11}$$

The convergence of the particle system to the Boltzmann equation can be understood as follows.

Theorem I.1 *[Lanford] There exists a time $T_L>0$ such that for any test function $h:\mathbb{T}^d\times\mathbb{R}^d\to\mathbb{R}$, any $\delta>0$ and $t\in[0,T_L]$,*

$$\mathbb{P}_\varepsilon\left(\left|\pi_t^\varepsilon(h) - \int_{\mathbb{T}^d\times\mathbb{R}^d} f(t,z)h(z)\right| > \delta\right) \xrightarrow[\mu_\varepsilon\to\infty]{} 0\,. \tag{12}$$

The time T_L depends only on the conditions (5) *for the smooth function f^0.*

Notice that stronger convergence statements can be found in [IP89, CIP94, GST14, PS17, Den18, BGSRS18, GG18, GG21]. All these studies rely on the BBGKY hierarchy and one of the goals of this paper is to provide an alternative derivation of Theorem I.1 by applying directly the cluster expansion at the level of the particle system.

To derive sharp estimates on the empirical measure, it is key to control its exponential moments, i.e. the Laplace transform

$$\Lambda_T^\varepsilon(e^h) := \frac{1}{\mu_\varepsilon}\log\mathbb{E}_\varepsilon\Big[\exp\Big(\mu_\varepsilon\,\pi_{[0,T]}^\varepsilon(h)\Big)\Big] = \frac{1}{\mu_\varepsilon}\log\mathbb{E}_\varepsilon\Big[\exp\Big(\sum_{i=1}^{\mathcal{N}} h\big(\mathbf{z}_i^\varepsilon([0,T])\big)\Big)\Big], \tag{13}$$

for test functions $h:\mathbb{D}([0,T],\mathbb{T}^d\times\mathbb{R}^d)\mapsto\mathbb{C}$ measuring informations on a single particle trajectory $\mathbf{z}^\varepsilon([0,T])$. Indeed, it is well known in probability theory that the large deviations can be related to the Legendre transform of $h\mapsto\Lambda_T^\varepsilon(e^h)$ and that the fluctuations are coded by the characteristic function which amounts to considering functions h with imaginary values. We refer to [BGSRS20c, BGSRS20a] for the derivation of the fluctuating Boltzmann equation and of the large deviations once the asymptotic behaviour of Λ_T^ε has been characterised.

In the rest of this paper, we first perform, in Section II, the dynamical cluster expansion to derive uniform controls on the exponential moments for fixed ε and then we analyse its Boltzmann-Grad limit in Section III. To illustrate this new approach, Theorem I.1 is recovered, in Section III B, without using the BBGKY hierarchy.

II. DYNAMICAL CLUSTER EXPANSION

A. The cluster expansion on trajectories

Throughout this section, we study the hard sphere dynamics on a fixed time interval $[0,T]$ and implement a cluster expansion to study the functional (13). We consider a test function h and assume that it satisfies the following bound uniformly on particle trajectories

$$\Big|\exp\Big(h\big(\mathbf{z}^\varepsilon([0,T])\big)\Big)\Big| \le c_1 \quad \text{for some fixed constant } c_1>0. \tag{14}$$

Simple examples to keep in mind are functions of the form

$$h\big(\mathbf{z}^\varepsilon([0,T])\big) := g_t\big(\mathbf{z}^\varepsilon(t)\big) \quad \text{or} \quad h\big(\mathbf{z}^\varepsilon([0,T])\big) := \int_0^T ds\, g_s\big(\mathbf{z}^\varepsilon(s)\big), \tag{15}$$

with $t \in [0,T]$ and bounded test functions $g_s : \mathbb{T}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ indexed by a time $s \in [0,T]$. Additional regularity assumptions on h (see (59)) will be needed later on in order to take the limit $\varepsilon \to 0$.

The exponential moment (13) can be reformulated in terms of the modified partition function

$$\mathcal{Z}^\varepsilon(e^h) := 1 + \sum_{N\geq 1} \frac{\mu_\varepsilon^N}{N!} \int_{\mathcal{D}_N^\varepsilon} dZ_N \prod_{i=1}^N f^0(z_i) \exp\Big(h(\mathbf{z}_i^\varepsilon([0,T]))\Big) \tag{16}$$

so that

$$\Lambda_T^\varepsilon(e^h) := \frac{1}{\mu_\varepsilon}\Big(\log \mathcal{Z}^\varepsilon(e^h) - \log \mathcal{Z}^\varepsilon(1)\Big)\,. \tag{17}$$

In order to rewrite $\log \mathcal{Z}^\varepsilon(e^h)$ as a tractable series expansion, we are going to introduce now several notations.

Even though the gas is extremely dilute in the Boltzmann-Grad asymptotics, particles are likely to interact dynamically. In this case their trajectories are strongly modified by scattering. Thus to implement the dynamical cluster expansion, a good point of view is to first group particles which have dynamical interactions during $[0,T]$ and then to perform the standard cluster expansion on these groups of particles. Classically, in statistical mechanics, these new objects are called polymers, but we will use the name forests to match the notations of [BGSRS20c]. @ Sergio, c'est plus general que le cas discret ?

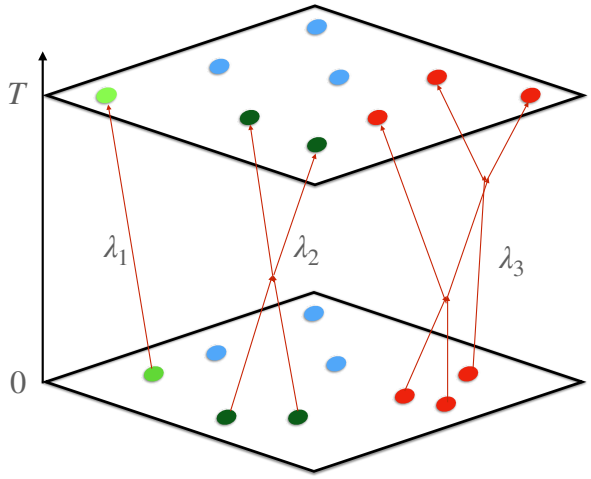

FIG. 1. On this figure, 3 forests $\lambda_1, \lambda_2, \lambda_3$ are depicted in the time interval $[0,T]$. They are formed by groups of particles interacting dynamically. As the forests do not intersect, the trajectories within a forest are only determined by the hard sphere dynamics restricted to the particles in this forest. Note that the other blue particles will form more forests which have not been represented.

Definition II.1 (Forest) *If two particles i, j collide during the time interval $[0,T]$, we say that they interact dynamically and write this condition $i \sim j$. The particles i, j are connected by a chain of dynamical interactions if there exists a collection of particles $i_1 = i, i_2, \dots, i_k = j$ such that $i_\ell \sim i_{\ell+1}$ for $\ell \leq k-1$.*

A forest λ is a collection of particle trajectories $\mathbf{Z}_\lambda^\varepsilon([0,T]) = \{z_i^\varepsilon([0,T])\}_{i\in\lambda}$ such that for any i, j in λ the particles i, j are connected by a chain of dynamical interactions within λ (see Figure 1). The notation λ will be used generically to represent the set of particles and the trajectories of the forest. The number of particles in the forest λ is denoted by $|\lambda|$. As the hard sphere dynamics is deterministic, the dynamical condition to form the forest λ is coded in the initial data which is denoted by Z_λ.

By construction, particles in a forest λ never collide with particles which do not belong to λ. Thus if a configuration $\mathbf{Z}_N^\varepsilon([0,T])$ is decomposed into a partition $\{\lambda_1, \dots, \lambda_k\}$ of forests then particles in different forests λ_i, λ_j do not collide. This condition is denoted by $\lambda_i \not\sim \lambda_j$. As a consequence, given the time interval $[0,T]$, the decomposition of $\mathbf{Z}_N^\varepsilon([0,T])$ into forests is unique and the forests are the maximally connected components keeping track of the particle dynamical interactions. The total kinetic energy of a forest λ_j is therefore time independent.

Using Definition II.1, any configuration of particle trajectories $\mathbf{Z}_N^\varepsilon([0,T])$ can be decomposed uniquely into a collection of forests so that

$$1 = \sum_{k\le N} \sum_{\{\lambda_1,\dots,\lambda_k\}\in \mathcal{P}^k_{\mathbf{Z}_N^\varepsilon}} \left(\prod_{j=1}^k \mathbf{1}_{\lambda_j \text{ forest}}\right)\left(\prod_{j\neq j'} \mathbf{1}_{\lambda_j\not\sim\lambda_{j'}}\right),$$

where $\mathcal{P}^k_{\mathbf{Z}_N^\varepsilon}$ is the set of partitions of the particle trajectories $\mathbf{Z}_N^\varepsilon([0,T])$ into k sets. As the dynamics is deterministic, fixing the initial data Z_N boils down to fixing the particle trajectories $\mathbf{Z}_N^\varepsilon([0,T])$ and therefore a forest decomposition. Thus plugging the previous identity in (16), we end up with

$$\mathcal{Z}^\varepsilon(e^h) := 1 + \sum_{N\ge 1} \frac{\mu_\varepsilon^N}{N!} \sum_{k\le N} \int_{\mathbb{T}^{dN}\times\mathbb{R}^{dN}} dZ_N \sum_{\{\lambda_1,\dots,\lambda_k\}\in \mathcal{P}^k_{\mathbf{Z}_N^\varepsilon}} \left(\prod_{j=1}^k \mathbf{1}_{\lambda_j \text{ forest}}\, F_T^{(h)}(\lambda_j)\right) \prod_{j\neq j'} \mathbf{1}_{\lambda_j\not\sim\lambda_{j'}}, \tag{18}$$

with a weight associated with each forest λ_j

$$F_T^{(h)}(\lambda_j) = \prod_{i=1}^{|\lambda_j|} f^0(z_i) \exp\left(h(\mathbf{z}_i^\varepsilon([0,T]))\right). \tag{19}$$

We stress the fact that, by definition of the forest λ_j, the particles in λ_j are not allowed to overlap initially

$$\forall i\neq i'\in\lambda_j, \qquad |x_i - x_{i'}|\ge\varepsilon,$$

otherwise the particle trajectories would be ill defined. The variables of interest are now the forests λ_j which encode the particle trajectories $\mathbf{Z}_{\lambda_j}^\varepsilon([0,T])$ constrained to collide during the time interval $[0,T]$.

Our goal is to rewrite (18) as the partition function of an interacting gas of forests. A given forest λ_j, with $|\lambda_j|$ particles and initial configuration Z_{λ_j}, is distributed according to the measure

$$d\boldsymbol{\nu}_T^{(h)}(\lambda_j) := \frac{\mu_\varepsilon^{|\lambda_j|}}{|\lambda_j|!} \mathbf{1}_{\lambda_j \text{ forest}}\, F_T^{(h)}(\lambda_j)\, dZ_{\lambda_j}, \tag{20}$$

where the support of the measure is restricted by the dynamical constraints so that the trajectories associated with the initial data Z_{λ_j} form a forest in the time interval $[0,T]$. This explains the dependence on T of the measure $\boldsymbol{\nu}_T^{(h)}$. Later on, the time T will be chosen small enough so that the gas of forests is diluted and the cluster expansion converges. Define also $d|\boldsymbol{\nu}_T^{(h)}|$ as in (20) with the modulus $|F_T^{(h)}|$ to take into account test functions h with complex values.

With these notations, the partition function (16) can be rewritten as a partition function of a gas of forests interacting by exclusion

$$\mathcal{Z}^\varepsilon(e^h) := 1 + \sum_{k\ge 1} \frac{1}{k!} \int d\boldsymbol{\nu}_T^{(h)}(\lambda_1)\dots d\boldsymbol{\nu}_T^{(h)}(\lambda_k) \prod_{j\neq j'} \mathbf{1}_{\lambda_j\not\sim\lambda_{j'}}, \tag{21}$$

where the integration for each forest is with respect to the number of particles in the forest as well as the initial coordinates of the particles (see (22)). This can be checked as follows. Starting from (18), a particle configuration Z_N is partitioned into k forests with cardinalities $n_1,\dots,n_k$

$$\begin{aligned}\mathcal{Z}^\varepsilon(e^h) &= 1 + \sum_{N\ge1} \frac{1}{N!} \sum_{k\le N} \frac{1}{k!} \sum_{\substack{n_1,\dots,n_k \\ n_1+\dots+n_k=N}} \frac{N!}{n_1!\dots n_k!} \mu_\varepsilon^{n_1+\dots+n_k} \int_{\mathbb{T}^{dN}\times\mathbb{R}^{dN}} \prod_{j=1}^k dZ_{\lambda_j} \prod_{j=1}^k \left(\mathbf{1}_{\substack{\lambda_j \text{ forest} \\ \text{of size } n_j}} F_T^{(h)}(\lambda_j)\right) \prod_{j\neq j'} \mathbf{1}_{\lambda_j\not\sim\lambda_{j'}} \\ &= 1 + \sum_{k\ge1} \frac{1}{k!} \int \prod_{j=1}^k dZ_{\lambda_j} \left(\sum_{n_j} \frac{\mu_\varepsilon^{n_j}}{n_j!} \mathbf{1}_{\substack{\lambda_j \text{ forest} \\ \text{of size } n_j}} F_T^{(h)}(\lambda_j)\right) \prod_{j\neq j'} \mathbf{1}_{\lambda_j\not\sim\lambda_{j'}},\end{aligned} \tag{22}$$

where the sums can be exchanged because the total number of particles in the box $\mathbb{T}^d$ is always finite for any fixed $\varepsilon>0$ thanks to the exclusion condition.

The main difficulty is to provide uniform estimates on $\mathcal{Z}^\varepsilon(e^h)$ with respect to ε in order to control the particle system in the Boltzmann-Grad limit. In the theory of cluster expansions, it is customary to control the exclusion interaction in (21)

$$\prod_{j\neq j'} \mathbf{1}_{\lambda_j\neq\lambda_{j'}} = \prod_{j\neq j'} \left(1-\mathbf{1}_{\lambda_j\sim\lambda_{j'}}\right)$$

by expanding the product above and then rearranging the terms. This requires to introduce further combinatorial decompositions. Let $\mathcal{G}_n$ the set of graphs with n vertices and $\mathcal{C}_n \subset \mathcal{G}_n$ the subset of connected graphs.

Definition II.2 (Overlap) *An overlap occurs between two forests $\lambda_j, \lambda_{j'}$ if two particles from $\mathbf{Z}^\varepsilon_{\lambda_j}([0,T])$ and $\mathbf{Z}^\varepsilon_{\lambda_{j'}}([0,T])$ are at a distance less than ε at some time in $[0,T]$. We will write $\lambda_j \sim \lambda_{j'}$. We stress the fact that an overlap between two forests does not change the dynamics of the forests : the particle trajectories remain encoded only by the particles within the forests (see Figure 2). In this sense, an overlap is a mathematical artefact which cannot be observed physically.*

A cluster of forests $\{\lambda_1,\dots,\lambda_k\}$ is formed by forests connected by chains of overlaps (by analogy with a chain of collisions in Definition II.1). It is associated with the combinatorial factor

$$\varphi(\lambda_1,\dots,\lambda_k) = \begin{cases} 1, & \text{if} \quad k=1, \\ \sum_{\mathcal{G}\in\mathcal{C}_k} \prod_{\{j,j'\}\in E(\mathcal{G})} (-\mathbf{1}_{\lambda_j\sim\lambda_{j'}}), & \text{if} \quad k\geq 2, \end{cases} \tag{23}$$

where the vertices of the graph $\mathcal{G}$ are indexed by forests and the product is over all the edges $E(\mathcal{G})$ of $\mathcal{G}$.

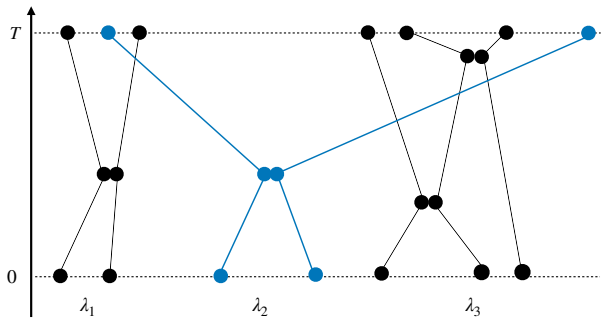

FIG. 2. On this figure, 3 forests $\lambda_1, \lambda_2, \lambda_3$ are depicted (the forest λ_2 is drawn in blue only for the sake of clarity). The particle dynamics inside each forest is not modified by an overlap. Notice that the forests λ_2, λ_3 overlap 3 times, this will be interpreted as a multiple edge in the dynamical correlation graph.

Within the previous framework, the cluster expansion theory (see e.g. [Uel04, PU09]) leads to

Proposition II.3 *There exists a time $T>0$ and a constant C such that uniformly in ε small enough and for $k\geq 1$*

$$\int d|\mathbf{v}_T^{(h)}|(\lambda_1)\dots d|\mathbf{v}_T^{(h)}|(\lambda_k)\ \varphi(\lambda_1,\dots,\lambda_k) \leq \mu_\varepsilon\ k!\ C^k\left(T+\varepsilon\right)^{k-1}. \tag{24}$$

This bounds holds uniformly for all h satisfying (14)*. Recall that the size of the forests is also an integration variable in* (24)*.*

As a consequence there is $T>0$ such that the cluster expansion converges uniformly for ε small enough

$$\log \mathcal{Z}^\varepsilon(e^h) := \sum_{k\geq 1} \frac{1}{k!} \int d\mathbf{v}_T^{(h)}(\lambda_1)\dots d\mathbf{v}_T^{(h)}(\lambda_k)\ \varphi(\lambda_1,\dots,\lambda_k). \tag{25}$$

The time T depends only on the initial data f^0 and on the constant c_1 in the upper bound (14) *on e^h.*

Note that the expansion (25) leads to a similar expansion for the Laplace transform defined in (17).

The time $T>0$ for the convergence of the cluster expansion is of the same order as the convergence time to the Boltzmann equation in Theorem I.1. In both cases, it is a fraction of the mean collision time between two particles. Indeed the requirement that the gas of forests is dilute means that the forest sizes have to remain small, i.e. that a particle cannot typically interact with too many particles. A crude analogy can be made with an Erdős-Renyi graph built by choosing randomly edges among N points with probability T/N. For $T<1$, this procedure leads with high probability to a collection of small graphs which corresponds to the dilute phase we have in mind for the hard sphere dynamics. Instead, as soon as $T>1$, a macroscopic connected graph appears.

We refer to [PSW16, PSW17, HP19] for refined statements on the generalisation of this dynamical phase transition in the case of particle dynamics. For this reason, we have made no attempt to optimise the time convergence $T > 0$ in Proposition II.3. Reaching longer time asymptotics requires new ideas and techniques. In Theorem I.1, the time restriction for the convergence of the iterated Duhamel series is also limited for similar technical reasons.

On pourrait faire une section heuristique plus tard sur les clusters et deplacer ce commentaire ?

Proof of Proposition II.3.

Assuming the validity of (24), the cluster expansion (25) follows from [Uel04]. We sketch the proof for the sake of completness. Expanding the exclusion in (21), we get

$$\mathcal{Z}^\varepsilon(e^h) = 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_k) \prod_{j \neq j'} \left(1 - \mathbf{1}_{\lambda_j \sim \lambda_{j'}}\right) = 1 + \sum_{k \geq 1} \frac{1}{k!} \int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_k) \sum_{\mathcal{G} \in \boldsymbol{\mathcal{G}}_k} \prod_{\{j,j'\} \in E(\mathcal{G})} \left(-\mathbf{1}_{\lambda_j \sim \lambda_{j'}}\right), \tag{26}$$

where the interactions between forests are now coded by graphs. Any graph $\mathcal{G} \in \boldsymbol{\mathcal{G}}_k$ can be decomposed into connected graphs $\mathcal{G} = \{\mathcal{G}_1, \dots, \mathcal{G}_n\}$ with $|\mathcal{G}_\ell| = m_\ell$ and $m_1 + \dots + m_n = k$. To do this, we partition $\{1, \dots, k\}$ into n sets and then enumerate the graphs on each set

$$\mathcal{Z}^\varepsilon(e^h) = 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n=1}^{k} \frac{1}{n!} \sum_{\substack{m_1, \dots, m_n \geq 1 \\ m_1 + \dots + m_n = k}} \frac{k!}{m_1! \dots m_n!} \prod_{\ell=1}^{n} \left(\int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_{m_\ell}) \sum_{\mathcal{G}_\ell \in \boldsymbol{\mathcal{C}}_{m_\ell}} \prod_{\{j,j'\} \in E(\mathcal{G}_\ell)} \left(-\mathbf{1}_{\lambda_j \sim \lambda_{j'}}\right) \right),$$

where $\frac{k!}{m_1! \dots m_n!}$ is the number of partitions into $\{m_1, \dots, m_n\}$ and $\frac{1}{n!}$ counts the multiplicity of $\{m_1, \dots, m_n\}$. For example for $k = 3, n = 2$, one has $(m_1 = 1, m_2 = 2)$ and $(m_1 = 2, m_2 = 1)$ which counts $n!$ times. Using the definition (23) of φ, we get

$$\mathcal{Z}^\varepsilon(e^h) = 1 + \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} 1_{n \leq k} \frac{1}{n!} \sum_{\substack{m_1, \dots, m_n \geq 1 \\ m_1 + \dots + m_n = k}} \prod_{\ell=1}^{n} \left(\int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_{m_\ell}) \frac{1}{m_\ell!} \varphi(\lambda_1, \dots, \lambda_{m_\ell}) \right).$$

Choosing T small enough, the sums are absolutely convergent thanks to (24) so that they can be swapped

$$\begin{aligned} \mathcal{Z}^\varepsilon(e^h) &= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{m_1, \dots, m_n \geq 1} \prod_{\ell=1}^{n} \left(\int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_{m_\ell}) \frac{1}{m_\ell!} \varphi(\lambda_1, \dots, \lambda_{m_\ell}) \right) \\ &= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\sum_{m \geq 1} \int d\boldsymbol{\nu}_T^{(h)}(\lambda_1) \dots d\boldsymbol{\nu}_T^{(h)}(\lambda_m) \frac{1}{m!} \varphi(\lambda_1, \dots, \lambda_m) \right)^n. \end{aligned}$$

This is the expansion of the exponential which can be inverted to recover (25).

We turn now to the derivation of (24) which relies on the specific structure of the microscopic dynamics and more precisely on the geometry of the trajectories in $[0, T]$. We will use the geometric estimates devised in [BGSRS20c] (see also [BGSRS20b]).

$\underline{k = 1.}$

We first consider a single forest λ_1 and prove the existence of a time $T > 0$ and of a constant C_0 such that

$$\int d|\boldsymbol{\nu}_T^{(h)}|(\lambda_1)\, e^{\frac{10}{\beta}|\lambda_1|} \leq C_0 \mu_\varepsilon, \tag{27}$$

where an additional term $e^{\frac{10}{\beta}|\lambda_1|}$ was added to inequality (24) for later purposes. Using the definition (20) of $\boldsymbol{\nu}_T^{(h)}$ and summing over the size n of the forest, one has

$$\int d|\boldsymbol{\nu}_T^{(h)}|(\lambda_1) e^{\frac{10}{\beta}|\lambda_1|} = \sum_{n \geq 1} \frac{\mu_\varepsilon^n}{n!} \int e^{\frac{10}{\beta} n} \left(\prod_{i=1}^{n} f^0(z_i) \left| \exp\left(h(\mathbf{z}_i^\varepsilon([0,T]))\right) \right| \right) \mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ forest}}\, dZ_n. \tag{28}$$

Thanks to assumption (5) on the initial distribution f^0 and assumption (14) on h, there is a constant $c > 0$ such that an upper bound can be derived in terms of the Gaussian measure (5) and the initial velocities

$$e^{\frac{10}{\beta} n} \prod_{i=1}^{n} f^0(z_i) \left| \exp\left(h(\mathbf{z}_i^\varepsilon([0,T]))\right) \right| \leq c^n\, \mathcal{M}_\beta^{\otimes n}(V_n). \tag{29}$$

Thus it is enough to show that there is $C > 0$ such that uniformly in $n \geq 2$

$$\int \mathcal{M}_{\beta/2}^{\otimes n}(V_n)\, \mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ forest } \lambda_1}\, dZ_n \leq n! \frac{C^n T^{n-1}}{\mu_\varepsilon^{n-1}}. \tag{30}$$

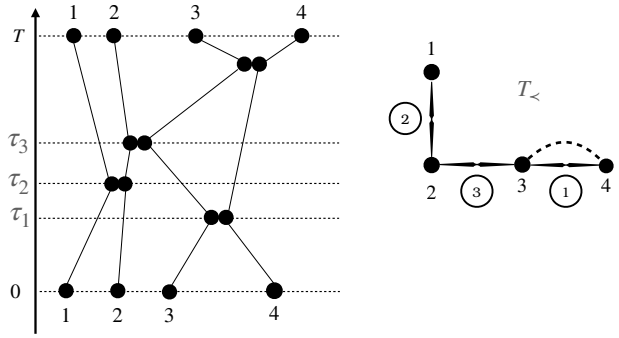

FIG. 3. A single forest with 4 particles ($n = 4$) is depicted on the left and the corresponding collision tree $\mathcal{T}_\prec$ is represented on the right. The edges of the tree $\mathcal{T}_\prec$ are ordered (circled numbers) according to the order of the collisions in the forest $\tau_1 < \tau_2 < \tau_3 \le T$. Recollisions may occur in the forest (as between particles 3 and 4 on the picture), but the corresponding (dashed) edge does not belong to $\mathcal{T}_\prec$. The collisions associated with the graph edges are called clustering collisions.

Note that only part of the Gaussian weight $\mathcal{M}_\beta^{\otimes n}$ in (29) has been used, as we shall need an additional exponential decay later on. By choosing $T > 0$ small enough, (27) is proven.

The constraint $\{\mathbf{Z}_n^\varepsilon \text{ forest}\}$ imposes that all the particles interact dynamically during the time interval $[0,T]$. We are going to record these collisions in an ordered tree $\mathcal{T}_\prec = (q_i, \bar{q}_i)_{1\le i\le n-1}$ (see Figure 3). There can be more than $n-1$ collisions in the dynamics, but in order to retain a minimal structure and to end up with a tree $\mathcal{T}_\prec$, the collisions creating a cycle in the graph are not recorded. The collisions kept in the tree $\mathcal{T}_\prec$ will be called *clustering collisions* : the first collision occurs between particles q_1 and $\bar{q}_1$ at time $\tau_1 \in [0,T]$, and the last collision is between q_{n-1} and $\bar{q}_{n-1}$ at time $\tau_{n-1} \in (\tau_{n-2}, T)$. In this way, an ordered graph recording the dynamical interactions is built by following the flow of the hard sphere dynamics in $[0,T]$. At intermediate times, the graph can be made of several connected components. The set of all oriented trees with n vertices is denoted by $\boldsymbol{\mathcal{T}}_n^\prec$. Thus summing over all the trees leads to

$$\mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ forest}} \le \sum_{\mathcal{T}_\prec \in \boldsymbol{\mathcal{T}}_n^\prec} \mathbf{1}_{\{Z_n \in \mathcal{R}_{\mathcal{T}_\prec}\}}\,, \tag{31}$$

where $\mathcal{R}_{\mathcal{T}_\prec}$ is the set of configurations Z_n with trajectories compatible with the ordered tree $\mathcal{T}_\prec$. By construction for any given Z_n coding a forest λ_1, only one term is non zero in the sum above.

For an admissible tree $\mathcal{T}_\prec$, the relative position, at the initial time, of the i^{th} colliding particles are denoted by

$$\hat{x}_i := x_{q_i} - x_{\bar{q}_i}\,. \tag{32}$$

Given the relative positions $(\hat{x}_j)_{j<i}$ and the velocities V_n, we consider a forward flow with clustering collisions at times $\tau_1 < \cdots < \tau_{i-1} < T$. By construction, q_i and $\bar{q}_i$ do not belong to the same connected component in the graph $G_{i-1} := (q_j, \bar{q}_j)_{1\le j\le i-1}$. We shall denote by $\mathcal{C}_{q_i}$ and by $\mathcal{C}_{\bar{q}_i}$ the connected components associated with $q_i, \bar{q}_i$ at time τ_{i-1}. Inside each connected component, the relative positions are fixed by the previous dynamical constraints, but the whole component can be translated so that a free parameter remains. Therefore by varying $\hat{x}_i$ (moving rigidly the connected components $\boldsymbol{\mathcal{C}}_{q_i}, \boldsymbol{\mathcal{C}}_{\bar{q}_i}$), a forward collision at time $\tau_i \in (\tau_{i-1}, T)$ between q_i and $\bar{q}_i$ can be triggered. This collision condition defines a set $\mathcal{B}_{\mathcal{T}_\prec,i}(\hat{x}_1, \dots, \hat{x}_{i-1}, V_n)$. If the particles q_i and $\bar{q}_i$ move in straight lines, then the collision at time τ_i imposes a constraint at time τ_{i-1}

$$\varepsilon = \left|\mathbf{x}_{q_i}^\varepsilon(\tau_i) - \mathbf{x}_{\bar{q}_i}^\varepsilon(\tau_i)\right| = \left|\mathbf{x}_{q_i}^\varepsilon(\tau_{i-1}) - \mathbf{x}_{\bar{q}_i}^\varepsilon(\tau_{i-1}) - (\tau_i - \tau_{i-1})\big(\mathbf{v}_{q_i}^\varepsilon(\tau_{i-1}^+) - \mathbf{v}_{\bar{q}_i}^\varepsilon(\tau_{i-1}^+)\big)\right|.$$

This says that the relative position at time τ_{i-1} has to belong to a tube of direction $\mathbf{v}_{q_i}^\varepsilon(\tau_{i-1}^+) - \mathbf{v}_{\bar{q}_i}^\varepsilon(\tau_{i-1}^+)$ with diameter ε and length $|\mathbf{v}_{q_i}^\varepsilon(\tau_{i-1}^+) - \mathbf{v}_{\bar{q}_i}^\varepsilon(\tau_{i-1}^+)|(T - \tau_{i-1})$ so that the collision occurs before time T. By moving rigidly the trajectories of the connected components associated with particles q_i and $\bar{q}_i$ at time τ_{i-1}, this imposes a condition on the initial relative position $\hat{x}_i$. Thus, the measure of the set $\mathcal{B}_{\mathcal{T}_\prec,i}$ is bounded from above by

$$|\mathcal{B}_{\mathcal{T}_\prec,i}| \le \frac{C}{\mu_\varepsilon} |\mathbf{v}_{q_i}^\varepsilon(\tau_{i-1}^+) - \mathbf{v}_{\bar{q}_i}^\varepsilon(\tau_{i-1}^+)| \int_{\tau_{i-1}}^T d\tau_i\,. \tag{33}$$

If the particle q_i (resp. $\bar{q}_i$) has been deflected during $[\tau_{i-1}, \tau_i[$ (by recollisions with particles in the connected component of $\boldsymbol{\mathcal{C}}_{q_i}$ (resp. $\boldsymbol{\mathcal{C}}_{\bar{q}_i}$)) then one has to decompose the trajectories into a union of tubes (as in Chapter 8 of [BGSRS20c]) and an estimate as above can be recovered. Averaging over all the possible pairs of particles, we get

$$\sum_{q_i,\bar{q}_i} |\mathcal{B}_{\mathcal{T}_\prec,i}| \le \frac{C}{\mu_\varepsilon} \left(V_n^2 + n\right) n \int_{\tau_{i-1}}^T d\tau_i\,, \tag{34}$$

where $V_n^2/2$ is the total kinetic energy of the particles in the forest λ_1. Since the collisions preserve the kinetic energy, V_n^2 is time independent.

Iterating the previous estimates, we get from Fubini's theorem

$$\sum_{\mathcal{T}_< \in \boldsymbol{\mathcal{T}}_n^<} \int d\hat{X}_n \prod_{i=1}^n \mathbf{1}_{\mathcal{B}_{\mathcal{T}_<,i}} \le \sum_{\mathcal{T}_< \in \boldsymbol{\mathcal{T}}_n^<} \int d\hat{x}_1 \mathbf{1}_{\mathcal{B}_{\mathcal{T}_<,1}} \int d\hat{x}_2 \cdots \int d\hat{x}_{n-1} \mathbf{1}_{\mathcal{B}_{\mathcal{T}_<,n-1}}$$
$$\le \left(\frac{C}{\mu_\varepsilon}\right)^{n-1} \left(V_n^2+n\right)^{n-1} n^{n-1} \int_0^T d\tau_1 \cdots \int_{\tau_{n-2}}^T d\tau_{n-1} \le \left(\frac{C}{\mu_\varepsilon}\right)^{n-1} \left(V_n^2+n\right)^{n-1} n^{n-1} \frac{T^{n-1}}{(n-1)!}, \tag{35}$$

where the last inequality follows by integrating the ordered times. Furthermore, for any K, N

$$\sup_{V \in \mathbb{R}^{dN}} \left\{ \exp\left(-\frac{\beta}{4}|V|^2\right) \left(|V|^2+K\right)^N \right\} \le C^N e^K N^N. \tag{36}$$

Using the Gaussian integration (30), we deduce from the previous inequality that the term $\left(V_n^2+n\right)^n$ leads to another factor of order n^n which is (up to a factor C^n) of the same order as $n!$. This completes (30) and thus (27).

$\underline{k>1.}$

We derive now (24) with k forests

$$\int d|\boldsymbol{v}_T^{(h)}|(\lambda_1) \dots d|\boldsymbol{v}_T^{(h)}|(\lambda_k)\, \varphi(\lambda_1,\dots,\lambda_k) \le \mu_\varepsilon\, k!\, C^k \left(T+\varepsilon\right)^{k-1}.$$

For this, we are going to use the inequality (27) which evaluates the constraints, in each forest λ_ℓ, on the coordinates of the particles Z_{λ_ℓ} at time 0. Further dynamical constraints are added by the function $\varphi(\lambda_1,\dots,\lambda_k)$ defined in (23). Viewing the overlaps between the forests as the edges of a graph with k vertices indexing the forests $\lambda_1,\dots,\lambda_k$, then the alternating sums defining $\varphi(\lambda_1,\dots,\lambda_k)$ can be bounded from above by the so called *tree inequality*

$$\left|\varphi(\lambda_1,\dots,\lambda_k)\right| \le \sum_{\mathcal{T}^{ov} \in \boldsymbol{\mathcal{T}}_k} 1_{\{\lambda_1,\dots,\lambda_k\} \hookrightarrow \mathcal{T}^{ov}}, \tag{37}$$

where the sum is restricted to (non-ordered) trees and the symbol $\{\lambda_1,\dots,\lambda_k\} \hookrightarrow \mathcal{T}^{ov}$ means that the graph coding the overlaps of $\{\lambda_1,\dots,\lambda_k\}$ contains the tree $\mathcal{T}^{ov}$. The tree inequality (37) which allows to control φ follows from a standard combinatorial argument (see [Pen67]) which will not be recalled here. Note that in (37), several graphs can be compatible with the same configuration so that several trees may contribute to the sum.

Since the particle trajectories are unchanged by the overlaps, it is not needed to proceed as for the collisions within the forests and to prescribe an order related to the dynamical overlaps on the edges of $\mathcal{T}^{ov}$. Thus, we choose an arbitrary order and examine successively the $k-1$ overlap constraints imposed on the forests. Denote by $\lambda_i, \bar{\lambda}_i$ the forests involved in the i^{th} overlap and by $q_i \in \lambda_i$ and $\bar{q}_i \in \bar{\lambda}_i$ the two overlapping particles. As for the collisions, the constraint imposed by the i^{th} overlap leads to a condition on the relative position of $q_i, \bar{q}_i$ at the initial time (see (32))

$$\hat{x}_i := x_{q_i} - x_{\bar{q}_i}.$$

Indeed, fixing the velocities in each forests, one has to evaluate the measure for the set $\left\{\hat{x}_i + \int_0^t ds \left(\mathbf{v}_{q_i}^\varepsilon(s) - \mathbf{v}_{\bar{q}_i}^\varepsilon(s)\right); \quad t \le T\right\}$ to intersect a ball of radius ε around the origin. We stress that the whole forests $\lambda_i, \bar{\lambda}_i$ move rigidly according to the positions $x_{q_i}, x_{\bar{q}_i}$. Note that, contrary to the collisions, the overlap may occur at the initial time or dynamically. This condition on $\hat{x}_i$ is coded by the set $\mathcal{B}_{\mathcal{T}^{ov},i}$ with measure bounded by

$$|\mathcal{B}_{\mathcal{T}^{ov},i}| \le C\varepsilon^d + \frac{C}{\mu_\varepsilon} \int_0^T ds\, |\mathbf{v}_{q_i}^\varepsilon(s) - \mathbf{v}_{\bar{q}_i}^\varepsilon(s)|. \tag{38}$$

We stress the fact that ε^d corresponds to the cost of an overlap at time 0 which is much smaller than the order of the cost $\frac{1}{\mu_\varepsilon} = \varepsilon^{d-1}$ of a dynamical overlap. This fact will be used in the Boltzmann-Grad limit to neglect the overlaps occurring at the initial time.

Denoting by $|\lambda|$ the cardinality of a forest and summing over all the possible particles in the forests $\lambda_i, \bar{\lambda}_i$, we get by a Cauchy-Schwarz inequality

$$\sum_{\substack{q_i \in \lambda_i, \\ \bar{q}_i \in \bar{\lambda}_i}} |\mathcal{B}_{\mathcal{T}^{ov},i}| \le \varepsilon^d\, |\lambda_i|\, |\bar{\lambda}_i| + \frac{C}{\mu_\varepsilon} \int_0^T ds \left(|\bar{\lambda}_i| \sqrt{|\lambda_i|} \sqrt{\sum_{q_i \in \lambda_i} |\mathbf{v}_{q_i}^\varepsilon(s)|^2} + |\lambda_i| \sqrt{|\bar{\lambda}_i|} \sqrt{\sum_{\bar{q}_i \in \bar{\lambda}_i} |\mathbf{v}_{\bar{q}_i}^\varepsilon(s)|^2} \right)$$
$$\le \varepsilon^d\, |\lambda_i|\, |\bar{\lambda}_i| + \frac{C}{\mu_\varepsilon} T \left(\frac{\beta}{4} V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\right)\left(\frac{\beta}{4} V_{\bar{\lambda}_i}^2 + \frac{4}{\beta}|\bar{\lambda}_i|\right) \le \frac{C}{\mu_\varepsilon} (T+\varepsilon) \left(\frac{\beta}{4} V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\right)\left(\frac{\beta}{4} V_{\bar{\lambda}_i}^2 + \frac{4}{\beta}|\bar{\lambda}_i|\right), \tag{39}$$

where we used in the 2nd inequality that the total kinetic energy $V_\lambda^2/2$ of the particles in a forest λ is constant in time. Thus (39) measures the cost of the overlap coded by the edge $(\lambda_i, \bar\lambda_i)$ in the tree $\mathcal{T}^{ov}$. As the particle trajectories are not modified by the overlaps, the conditions imposed by the $k-1$ overlaps can be successively satisfied by moving rigidly the forests. Let $\mathcal{B}_{\mathcal{T}^{ov}}$ be the set representing all the conditions imposed by the overlaps. Given $\{V_{\lambda_1}, \dots, V_{\lambda_k}\}$ the initial velocities of all the particles, the measure of $\mathcal{B}_{\mathcal{T}^{ov}}$ with respect to the positions is obtained by multiplying the contributions (39) for each edge of the tree $\mathcal{T}^{ov}$

$$|\mathcal{B}_{\mathcal{T}^{ov}}| \le \left(\frac{C}{\mu_\varepsilon}\right)^{k-1} (T+\varepsilon)^{k-1} \prod_{i=1}^{k} \Big(\frac{\beta}{4} V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\Big)^{d_i},$$

where d_i stands for the degree of the vertex λ_i in the tree $\mathcal{T}^{ov}$. There are $(k-2)!/\prod_i (d_i-1)!$ trees of size k with specified vertex degrees (see e.g. Lemma 2.4.1 in [BGSRS20c]). Thus summing over all the trees $\mathcal{T}^{ov}$, we get

$$\begin{aligned}\sum_{\mathcal{T}^{ov}\in\boldsymbol{\mathcal{T}}_k} |\mathcal{B}_{\mathcal{T}^{ov}}| &\le \left(\frac{C}{\mu_\varepsilon}\right)^{k-1} (T+\varepsilon)^{k-1}(k-2)! \sum_{\substack{d_1,\dots d_k \\ d_1+\dots d_k = 2k-2}} \prod_{i=1}^{k} \frac{\Big(\frac{\beta}{4}V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\Big)^{d_i}}{(d_i-1)!} \\ &\le \left(\frac{C}{\mu_\varepsilon}\right)^{k-1} (T+\varepsilon)^{k-1}(k-2)! \prod_{i=1}^{k} \left(\frac{\beta}{4}V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\right) \exp\left(\frac{\beta}{4}V_{\lambda_i}^2 + \frac{4}{\beta}|\lambda_i|\right),\end{aligned}$$

where the constraint on the degrees is released in the last inequality to recover the exponential.

Using the Gaussian weights $\mathcal{M}_{\beta/2}^{\otimes|\lambda_i|}$ from the initial measure as well as the inequality (36), we obtain an upper bound for the overlaps of the form

$$\sum_{\mathcal{T}^{ov}\in\boldsymbol{\mathcal{T}}_k} |\mathcal{B}_{\mathcal{T}^{ov}}| \prod_{i=1}^{k} \mathcal{M}_{\beta/2}^{\otimes|\lambda_i|}(Z_{|\lambda_i|}) \le \frac{C^k}{\mu_\varepsilon^{k-1}} k! (T+\varepsilon)^{k-1} \prod_{i=1}^{k} e^{\frac{10}{\beta}|\lambda_i|}. \tag{40}$$

Once the dynamical constraint on the overlaps has been taken into account, the contributions of the forests are independent and can be estimated by (27) for T small enough

$$\prod_{i=1}^{k} \int d|\boldsymbol{v}_T^{(h)}|(\lambda_i)\, e^{\frac{10}{\beta}|\lambda_i|} \le C_0^k \mu_\varepsilon^k. \tag{41}$$

Combining (40) and (41), we deduce that

$$\int d|\boldsymbol{v}_T^{(h)}|(\lambda_1) \dots d|\boldsymbol{v}_T^{(h)}|(\lambda_k)\, \varphi(\lambda_1,\dots,\lambda_k) \le \mu_\varepsilon\, k!\, C^k\, (T+\varepsilon)^{k-1}. \tag{42}$$

This completes the proof of (24) for a value of $T>0$ small enough so that (27) holds.

B. Correlations & cumulants

Recalling (17), we deduce from the cluster expansion of Proposition II.3 that there exists $T>0$ such that the Laplace transform

$$\begin{aligned}\Lambda_T^\varepsilon(e^h) &= \frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon\Big[\exp\Big(\mu_\varepsilon\, \pi_{[0,T]}^\varepsilon(h)\Big)\Big] = \frac{1}{\mu_\varepsilon}\log\left(\frac{\mathcal{Z}^\varepsilon(e^h)}{\mathcal{Z}^\varepsilon(1)}\right) \\ &= \frac{1}{\mu_\varepsilon}\sum_{k\ge1}\frac{1}{k!}\left(\int d\boldsymbol{v}_T^{(h)}(\lambda_1)\dots d\boldsymbol{v}_T^{(h)}(\lambda_k)\, \varphi(\lambda_1,\dots,\lambda_k) - \int d\boldsymbol{v}_T^{(0)}(\lambda_1)\dots d\boldsymbol{v}_T^{(0)}(\lambda_k)\, \varphi(\lambda_1,\dots,\lambda_k)\right)\end{aligned}$$

can also be expanded as a series. In particular $h \mapsto \Lambda_T^\varepsilon(e^h)$ is analytic in a L^∞-neighbourhood of 0. il me semble que L^∞ suffit pour ce qu'on veut dans cette section This is an important property as the derivatives of the functional are related to physical quantities. Indeed considering the first derivative at 0 of $u \in \mathbb{R} \mapsto \Lambda_T^\varepsilon(e^{uh})$, we recover the expectation of the empirical measure (using the notation of (13))

$$\mathbb{E}_\varepsilon\Big[\pi_{[0,T]}^\varepsilon(h)\Big] = \partial_u \Lambda_T^\varepsilon(e^{uh})\Big|_{u=0} = \frac{1}{\mu_\varepsilon}\sum_{k\ge1}\frac{1}{k!}\int d\boldsymbol{v}_T^{(0)}(\lambda_1)\dots d\boldsymbol{v}_T^{(0)}(\lambda_k)\, \varphi(\lambda_1,\dots,\lambda_k)\left(\sum_{\ell=1}^{k}\sum_{i\in\lambda_\ell} h\big(\mathbf{z}_i^\varepsilon([0,T])\big)\right). \tag{43}$$

In particular, the density at time $t \in [0,T]$ can be obtained by using test functions of the form $h\big(\mathbf{z}^\varepsilon([0,T])\big) = h\big(\mathbf{z}^\varepsilon(t)\big)$. This series will be used in Section III B to recover the Boltzmann equation.

Taking twice the derivative leads to the variance

$$\mathbb{E}_\varepsilon\left[\pi^\varepsilon_{[0,T]}(h)^2\right] - \mathbb{E}_\varepsilon\left[\pi^\varepsilon_{[0,T]}(h)\right]^2 = \frac{1}{\mu_\varepsilon}\partial_u^2 \Lambda^\varepsilon_T(e^{uh})\Big|_{u=0}. \tag{44}$$

Adapting the proof of (24), we deduce that the second derivative is uniformly bounded wrt ε

$$\begin{aligned}\partial_u^2 \Lambda^\varepsilon_T(e^{uh})\Big|_{u=0} &= \frac{1}{\mu_\varepsilon}\sum_{k\geq 1}\frac{1}{k!}\int d\boldsymbol{\nu}_T^{(0)}(\lambda_1)\dots d\boldsymbol{\nu}_T^{(0)}(\lambda_k)\,\varphi(\lambda_1,\dots,\lambda_k)\left(\sum_{\ell=1}^k\sum_{i\in\lambda_\ell} h\big(\mathbf{z}_i^\varepsilon([0,T])\big)\right)^2 \\ &\leq \|h\|_\infty^2\frac{1}{\mu_\varepsilon}\sum_{k\geq 1}\frac{1}{k!}\int d|\boldsymbol{\nu}_T^{(0)}|(\lambda_1)\dots d|\boldsymbol{\nu}_T^{(0)}|(\lambda_k)\,\varphi(\lambda_1,\dots,\lambda_k)\left(\sum_{\ell=1}^k|\lambda_\ell|\right)^2 \leq C.\end{aligned} \tag{45}$$

This implies that the covariance vanishes in the Boltzmann-Grad limit so that the empirical measure concentrates to its mean

$$\mathbb{E}_\varepsilon\left[\left(\pi^\varepsilon_{[0,T]}(h) - \mathbb{E}_\varepsilon\left[\pi^\varepsilon_{[0,T]}(h)\right]\right)^2\right] = \mathbb{E}_\varepsilon\left[\pi^\varepsilon_{[0,T]}(h)^2\right] - \mathbb{E}_\varepsilon\left[\pi^\varepsilon_{[0,T]}(h)\right]^2 = \frac{1}{\mu_\varepsilon}\partial_u^2\Lambda^\varepsilon_T(e^{uh})\Big|_{u=0} = O\left(\frac{\|h\|_\infty^2}{\mu_\varepsilon}\right). \tag{46}$$

Expanding (46) and using the symmetry between particles, we deduce also that the particle trajectories are asymptotically independent

$$\mathbb{E}_\varepsilon\left[h\big(\mathbf{z}_1^\varepsilon([0,T])\big)h\big(\mathbf{z}_2^\varepsilon([0,T])\big)\right] - \mathbb{E}_\varepsilon\left[h\big(\mathbf{z}_1^\varepsilon([0,T])\big)\right]^2 = O\left(\frac{\|h\|_\infty^2}{\mu_\varepsilon}\right). \tag{47}$$

This property is often called propagation of chaos.

By taking further derivatives, one can recover all the cumulants and show that the L^1-norm of the cumulant of order n decays as $O\big(\mu_\varepsilon^{1-n}\big)$. This result was already obtained in [BGSRS20c] (see Theorem 4 therein). Notice however that the series expansion for $\Lambda^\varepsilon_T(e^h)$ is derived in [BGSRS20c] by applying cluster expansion on the Duhamel representation of the correlation functions and the terms of the series are described by pseudo-trajectories instead of physical trajectories. Nevertheless the expansions in this paper and in [BGSRS20c] provide the same results (with different times T).

III. BOLTZMANN-GRAD LIMIT

The estimates derived in the previous section hold uniformly with respect to ε (small enough). In this section, we are going focus on the kinetic limit $\varepsilon \to 0$.

A. Limiting cluster expansion

The series expansion of the partition function $\log \mathcal{Z}^\varepsilon(e^h)$, in Proposition II.3, is coded by the dynamical interactions of microscopic trajectories. We are going to show that the structure of these interactions simplifies in the Boltzmann-Grad limit, providing a simpler (but singular) expansion for the limit of $\Lambda^\varepsilon_T(e^h)$ (see Proposition III.3).

1. Discarding recollisions and overlap

We first consider the dynamical interactions within a forest λ_1 of size n and show that, in the Boltzmann-Grad limit, the only relevant trajectories have exactly $n-1$ collisions. Recall that in a microscopic configuration compatible with this forest $\mathbf{Z}^\varepsilon_{\lambda_1}$, all the particles interact dynamically in the sense of Definition II.1. All these interactions can be recorded in a graph $\mathcal{G}$ with n vertices labelled by the particles and edges corresponding to a collision between two particles. By definition of the forest λ_1, the graph $\mathcal{G}$ will be connected and it may have cycles or multiple edges (see Figure 4). These loops correspond to recollisions in the hard sphere dynamics starting from the configuration Z_n. We stress the fact that this notion of recollision slightly differs from the interpretation of recollisions used in the Duhamel representation [CIP94, Spo81, PS17, BGSRS20c]. Indeed, in the latter case, the recollisions refer to pseudo-trajectories and one has to distinguish between the internal recollisions (which can be neglected) and the external recollisions (which are relevant for the cumulants [BGSRS20c]). In our setting, the forests are determined by

the physical microscopic dynamics and all the recollisions are negligible in the Boltzmann-Grad limit. In particular, the only relevant graphs will be trees, i.e. minimally connected graphs. In this case, we say that λ_1 is a *0-forest* and the corresponding reduced distribution is restricted to particle configurations compatible with this condition

$$d\boldsymbol{\nu}_T^{(h),0}(\lambda_1) = \frac{\mu_\varepsilon^{|\lambda_1|}}{|\lambda_1|!} F_T^{(h)}(\lambda_1)\, \mathbf{1}_{\lambda_1 \text{ 0-forest}}\, dZ_{\lambda_1}. \tag{48}$$

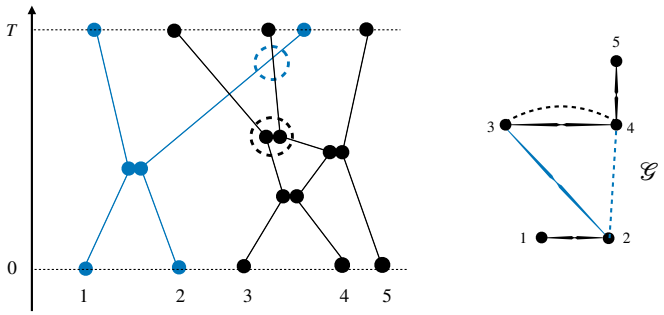

FIG. 4. On the left, two overlapping forests are represented with different colors. The dynamical graph of interactions is depicted on the right with black edges for the collisions and blue edges for the overlaps. The minimal dynamical graph corresponds to the arrows, instead the recollisions and multiple overlaps are represented by dashed edges.

In the proof of Proposition II.3, Estimate (27), recalled below,

$$\int d|\boldsymbol{\nu}_T^{(h)}|(\lambda_1)\, e^{\frac{10}{\beta}|\lambda_1|} \le C_0 \mu_\varepsilon$$

was derived by showing that the collisions between particles in a forest can be indexed by a tree. This tree records the minimal amount of dynamical contraints and the recollisions add more contraints which can be controled by the geometric estimates derived in [BGSRS20b] (see Eq (5.12) and Appendix B), leading to

$$\Big| \int d\boldsymbol{\nu}_T^{(h),0}(\lambda_1)\, e^{\frac{10}{\beta}|\lambda_1|} - \int d\boldsymbol{\nu}_T^{(h)}(\lambda_1)\, e^{\frac{10}{\beta}|\lambda_1|} \Big| \le C\, \mu_\varepsilon\, \varepsilon^{\alpha_d}, \tag{49}$$

for some constant $\alpha_d > 0$ depending on the dimension and T small enough as in Proposition II.3. pour la dimension 2, que dit-on ?

The second source of dynamical interactions is due to overlaps. We consider now k overlapping forests $\lambda_1, \dots, \lambda_k$. The combinatorial factor $\varphi(\lambda_1, \dots, \lambda_k)$ has been estimated in (37), recalled below, as an upper bound on trees with edges between two overlapping forests

$$\big|\varphi(\lambda_1, \dots, \lambda_k)\big| \le \sum_{\mathcal{T}^{ov} \in \boldsymbol{\mathcal{T}}_k} 1_{\{\lambda_1, \dots, \lambda_k\} \hookrightarrow \mathcal{T}^{ov}}.$$

If the graph recording all the overlaps has cycles, then several trees will contribute to the sum above. As for the recollisions, we can show that cycles can be neglected in the limit and that typically the constraint $\varphi(\lambda_1, \dots, \lambda_k)$ is compatible with a single tree. Furthermore, as noted in the comment after (38), the overlaps occurring initially have a much smaller cost than the dynamical overlaps. Thus they can also be neglected in the Boltzmann-Grad limit.

In the following, we shall denote by $\{\lambda_1, \dots, \lambda_k\} \longmapsto \mathcal{T}^{ov}$ the constraint that the overlaps are compatible with a single tree $\mathcal{T}^{ov}$ and that there is no overlap at the initial time. In other words, the graph on k vertices coding all the different overlaps between the forests has no cycles (note that if two forests overlap several times, as on Figure 4, this is counted only as one edge in such graph; i.e. multiple edges are disregarded). As the tree $\mathcal{T}^{ov}$ has $k-1$ edges, the reduced overlap function takes the value $(-1)^{k-1}$ and is defined by (recall (23))

$$\varphi^0(\lambda_1, \dots, \lambda_k) := (-1)^{k-1} \sum_{\mathcal{T}^{ov} \in \boldsymbol{\mathcal{T}}_k} 1_{\{\lambda_1, \dots, \lambda_k\} \longmapsto \mathcal{T}^{ov}}, \tag{50}$$

where at most one term in the sum above is not equal to 0.

Combining the proof of Proposition II.3 and the geometric estimates derived in [BGSRS21], one can show that the overlaps forming cycles do not contribute in the Boltzmann-Grad limit. As the recollisions can also be neglected thanks to (49), we finally obtain that the minimally connected graphs provide the leading contribution to the cluster expansion series.

Proposition III.1 *Let $T>0$ be the convergence time obtained in Proposition II.3. There is are constants $C,\alpha_d>0$ such that for uniformly in ε small enough and for $k\geq 1$*

$$\left|\int d\boldsymbol{v}_T^{(h),0}(\lambda_1)\dots d\boldsymbol{v}_T^{(h),0}(\lambda_k)\,\varphi^0(\lambda_1,\dots,\lambda_k)-\int d\boldsymbol{v}_T^{(h)}(\lambda_1)\dots d\boldsymbol{v}_T^{(h)}(\lambda_k)\,\varphi(\lambda_1,\dots,\lambda_k)\right|\leq \mu_\varepsilon\,\varepsilon^{\alpha_d}\,k!\,C^k(T+\varepsilon)^{k-1}. \tag{51}$$

As a consequence, there is $T>0$ such that

$$\left|\log\mathcal{Z}^\varepsilon(e^h)-\sum_{k\geq 1}\frac{1}{k!}\int d\boldsymbol{v}_T^{(h),0}(\lambda_1)\dots d\boldsymbol{v}_T^{(h),0}(\lambda_k)\,\varphi^0(\lambda_1,\dots,\lambda_k)\right|\leq C\,\mu_\varepsilon\,\varepsilon^{\alpha_d}. \tag{52}$$

For fixed k, the term $\int d\boldsymbol{v}_T^{(h),0}(\lambda_1)\dots d\boldsymbol{v}_T^{(h),0}(\lambda_k)\,\varphi^0(\lambda_1,\dots,\lambda_k)$ in (51) can be rewritten in a different way. Given $\{\lambda_1,\dots,\lambda_k\}$ a set of overlapping forests, the corresponding particle configuration will be linked by $|\lambda_\ell|-1$ collisions in each forest λ_ℓ and $k-1$ overlaps between forests. In particular, if n stands for the total number of particles in $\{\lambda_1,\dots,\lambda_k\}$, we say that there are

$$n-1=\sum_{\ell=1}^{k}(|\lambda_\ell|-1)+k-1.$$

clustering conditions (generalizing the clustering collisions introduced at the level of (31)). Ordering all these clustering conditions according to the forward flow, they can be indexed by a single signed ordered tree $\overline{\mathcal{T}}_\prec$ such that the n particles form the vertices and each edge e has a sign $s_e=+1$ if it records a collision or $s_e=-1$ if it records an overlap. Thus instead of decomposing the particles into overlapping forests, one can choose globally a set of n particles and signed ordered trees $\overline{\mathcal{T}}_\prec$ to code the clustering conditions. By the Fubini Theorem, we deduce that

$$\sum_{k\geq 1}\frac{1}{k!}\int d\boldsymbol{v}_T^{(h),0}(\lambda_1)\dots d\boldsymbol{v}_T^{(h),0}(\lambda_k)\,\varphi^0(\lambda_1,\dots,\lambda_k)=\sum_{n=1}^{\infty}\frac{\mu_\varepsilon^n}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int dZ_n\,F_T^{(h)}(\mathbf{Z}_n^\varepsilon)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon\text{ 0-forest compatible with }\overline{\mathcal{T}}_\prec}, \tag{53}$$

where $\boldsymbol{\mathcal{T}}_n^{\prec,\pm}$ is the set of signed ordered trees with n vertices and $F_T^{(h)}(\mathbf{Z}_n^\varepsilon)$ is defined as in (19).

2. *Asymptotics of the partition function*

We are going to use Proposition III.1 to compute the asymptotic of the partition function when μ_ε tends to infinity. In the Boltzmann-Grad limit, the particle trajectories in the series expansion (53) become singular, but a limiting structure can be identified provided the integration parameters are properly reindexed.

Given n and a signed ordered tree $\overline{\mathcal{T}}_\prec$, we consider the particle trajectories in the term of order n of (53). For fixed $\varepsilon>0$, the clustering condition associated with the edge $e=\{i,j\}$ takes the form

$$\omega_e:=\frac{x_i(\tau_e)-x_j(\tau_e)}{\varepsilon}\in\mathbb{S}^{d-1}, \tag{54}$$

where the clustering (collision or overlap) time is denoted by τ_e. We recall that the overlaps occurring at time 0 have been discarded in Proposition III.1 so that all the clusterings occur only dynamically. Recall that before the clustering, the particles i,j are connected to two distinct components of the dynamical graph which can move rigidly with respect to the positions of i and j at time zero. Fixing (x_i,v_i,v_j) at time τ_e^- and the configurations inside each dynamical components associated with i and j, we consider the local change of variables

$$x_j\in\mathbb{T}^d\mapsto(\tau_e,\omega_e)\in[0,t]\times\mathbb{S}^{d-1} \tag{55}$$

with Jacobian $\mu_\varepsilon^{-1}\big((v_i-v_j)\cdot\omega_e\big)_+$. This provides the identification of measures

$$\mu_\varepsilon\,dx_i\,dv_i\,dx_j\,dv_j=dx_i\,dv_i\,dv_j\,d\tau_e\,d\omega_e\big((v_i(\tau_e^-)-v_j(\tau_e^-))\cdot\omega_e\big)_+. \tag{56}$$

Applying this change of variables for each edge of the clustering tree $\overline{\mathcal{T}}_\prec$ in a decreasing order, a trajectory configuration $\mathbf{Z}_n^\varepsilon([0,T])$ can be built by the following parameters c'est un peu de gymnastique, faut-il commenter ? :

- (x_1,v_1) the coordinates of particle 1 at time 0,
- $(v_2,\dots,v_n)$ the particle velocities at the initial time,

- $\Omega_{n-1} = (\omega_e)_{e\in E(\overline{\mathcal{T}}_\prec)}$ representing the clustering vectors,
- $\Theta_{n-1} = (\tau_e)_{e\in E(\overline{\mathcal{T}}_\prec)}$ representing the clustering times,
- $\Sigma_{n-1} = (s_e)_{e\in E(\overline{\mathcal{T}}_\prec)}$ which are equal to 1 if a collision occurs and -1 for an overlap.

We define the limiting singular measure

$$d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}\big(\mathbf{Z}_n^\varepsilon\big) := dx_1 dV_n\, d\Theta_{n-1}\, d\Omega_{n-1} \prod_{e=\{i,j\}\in E(\overline{\mathcal{T}}_\prec)} s_e\Big(\big(v_i(\tau_e^-)-v_j(\tau_e^-)\big)\cdot\omega_e\Big)_+, \tag{57}$$

where the clustering times are ordered according to the edges in the tree. Note that for simplicity, the measure is indexed by the trajectories $\mathbf{Z}_n^\varepsilon := \mathbf{Z}_n^\varepsilon([0,T])$ which, for a given tree $\overline{\mathcal{T}}_\prec$, are in one-to-one with the parameters $(x_1, V_n, \Theta_{n-1}, \Omega_{n-1})$. Iterating the change of variables (56) for the $n-1$ clustering conditions prescribed by a given tree $\overline{\mathcal{T}}_\prec$, one gets

$$\mu_\varepsilon^{n-1}\int dZ_n\, F_T^{(h)}(\mathbf{Z}_n^\varepsilon)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ 0-forest compatible with } \overline{\mathcal{T}}_\prec} = \int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}\big(\mathbf{Z}_n^\varepsilon\big)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ 0-forest}} \prod_{i=1}^n f^0\big(\mathbf{z}_i^\varepsilon(0)\big)\exp\Big(h\big(\mathbf{z}_i^\varepsilon([0,T])\big)\Big). \tag{58}$$

The parameters drawn from the measure $d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}$ do not depend on ε, thus for some values of ε the corresponding trajectory $\mathbf{Z}_n^\varepsilon$ may not form a 0-forest and the indicator function in the RHS of (58) imposes this compatibility constraint.

Given a signed tree $\overline{\mathcal{T}}_\prec$ and parameters $(x_1, V_n, \Theta_{n-1}, \Omega_{n-1})$, the configuration $\mathbf{Z}_n^\varepsilon([0,T])$ converges, when ε tends to 0, to a limiting configuration $\mathbf{Z}_n([0,T])$ such that the particles coincide at the clustering times as in the definition below.

Definition III.2 (Limiting trajectories) *Fix a signed ordered tree $\overline{\mathcal{T}}_\prec$ of size n and a collection of parameters $(x_1, V_n, \Theta_{n-1}, \Omega_{n-1})$ as in* (57)*. The corresponding limiting trajectory can be constructed as follows. In between two clustering times, all particles evolve according to the forward free flow and for each edge $e = (i,j) \in \overline{\mathcal{T}}_\prec$, the corresponding constraints are imposed at the clustering time τ_e:*

- *a collision occurs if $s_e = 1$ (resp. an overlap occurs if $s_e = -1$) between the particles i, j,*
- *the positions of both particles coincide $x_i(\tau_e) = x_j(\tau_e)$,*
- *if $s_e = +1$, then the velocities $v_i(\tau_e^+)$ and $v_j(\tau_e^+)$ are scattered according to the rule* (9) *with scattering vector ω_e.*

A limiting trajectory on the time interval $[0,T]$ is denoted by $\mathbf{Z}_n([0,T]) = \big(z_i([0,T])\big)_{i\le n}$. In the following, it will be convenient to use the shorthand $\mathbf{Z}_n$.

Finally, we can state the regularity assumption needed on the test function h to take the Boltzmann-Grad limit. We assume that the test function $h : \mathbb{D}([0,T], \mathbb{T}^d\times\mathbb{R}^d) \to \mathbb{C}$ satisfies the bound (14) and that for all tree $\overline{\mathcal{T}}_\prec$ and almost all parameters $(x_1, V_n, \Theta_{n-1}, \Omega_{n-1})$, the following limit holds

$$\lim_{\varepsilon\to 0}\sum_{i=1}^n h\big(\mathbf{z}_i^\varepsilon([0,T])\big) = \sum_{i=1}^n h\big(\mathbf{z}_i([0,T])\big). \tag{59}$$

Notice that $\mathbf{Z}_n^\varepsilon([0,T])$ tends to $\mathbf{Z}_n([0,T])$ with respect to the Skorohod distance which is well suited to handle piecewise continuous functions (see [Bil99]). Thus a natural assumption would have been the continuity of h with respect to the Skorohod topology. However this is not sufficient to cover all cases of interest, in particular a test function of the form $h\big(\mathbf{z}([0,T])\big) := g(\mathbf{z}(t))$ (with g a continuous function $\mathbb{T}^d\times\mathbb{R}^d$) is continuous only at trajectories without jumps at time t. This is why the convergence (59) is only required almost surely.

By Proposition III.1, we know that the cycles have a vanishing probability when ε goes to 0 so that for all tree $\overline{\mathcal{T}}_\prec$ and almost all parameters $(x_1, V_n, \Theta_{n-1}, \Omega_{n-1}, \Sigma_{n-1})$, one has also

$$\lim_{\varepsilon\to 0}\mathbf{1}_{\mathbf{Z}_n^\varepsilon \text{ 0-forest}} = 1. \tag{60}$$

The limit of the functional Λ_T^ε defined in (13) can be formulated in terms of the limiting trajectories and Theorem 6 of [BGSRS20c] is recovered below.

Proposition III.3 *Let $T>0$ be the convergence time obtained in Proposition II.3. Then the following limit holds*

$$\lim_{\varepsilon\to 0}\Lambda_T^\varepsilon(e^h)=\Lambda_T(e^h):=-1+\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\prod_{i=1}^{n}f^0\big(z_i(0)\big)\exp\Big(h\big(z_i([0,T])\big)\Big). \tag{61}$$

Furthermore the limiting functional $h\mapsto\Lambda_T(e^h)$ is analytic for h satisfying (14) *as the series is absolutely convergent*

$$\left|\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\prod_{i=1}^{n}f^0\big(z_i(0)\big)\exp\Big(h\big(z_i([0,T])\big)\Big)\right|\le C^n\,T^{n-1}. \tag{62}$$

Proof.

We know from (17) that $\Lambda_T^\varepsilon(e^h):=\frac{1}{\mu_\varepsilon}\big(\log\mathcal{Z}^\varepsilon(e^h)-\log\mathcal{Z}^\varepsilon(1)\big)$. Thus it is enough to compute the limit of each partition function. Combining (52) and (53), this boils down to studying the asymptotics of each term of the series

$$\left|\frac{1}{\mu_\varepsilon}\log\mathcal{Z}^\varepsilon(e^h)-\sum_{n=1}^{\infty}\frac{\mu_\varepsilon^{n-1}}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int dZ_n\;F_T^{(h)}(\mathbf{Z}_n^\varepsilon)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon}\text{ 0-forest compatible with }\overline{\mathcal{T}}_\prec\right|\le C\,\varepsilon^{\alpha_d},$$

as the series is absolutely convergent, uniformly in ε small enough, by the same estimates as in the proof of Proposition II.3 :

$$\left|\frac{\mu_\varepsilon^{n-1}}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int dZ_n\;F_T^{(h)}(\mathbf{Z}_n^\varepsilon)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon}\text{ 0-forest compatible with }\overline{\mathcal{T}}_\prec\right|\le C^n\,T^{n-1}. \tag{63}$$

Changing variables as in (58), the term of order n in the series becomes

$$\begin{aligned}&\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\mu_\varepsilon^{n-1}\int dZ_n\;F_T^{(h)}(\mathbf{Z}_n^\varepsilon)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon}\text{ 0-forest compatible with }\overline{\mathcal{T}}_\prec \\ &\quad=\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}\big(\mathbf{Z}_n^\varepsilon\big)\,\mathbf{1}_{\mathbf{Z}_n^\varepsilon}\text{ 0-forest}\prod_{i=1}^{n}f^0\big(\mathbf{z}_i^\varepsilon(0)\big)\exp\Big(h\big(\mathbf{z}_i^\varepsilon([0,T])\big)\Big).\end{aligned} \tag{64}$$

Given the collection of parameters $(x_1,V_n,\Theta_{n-1},\Omega_{n-1})$, a trajectory configuration $\mathbf{Z}_n^\varepsilon([0,T])$ has a pointwise limit $\mathbf{Z}_n([0,T])$ when ε tends to 0. Recall that f^0 is continuous and the integrand is bounded from above by (29), thus the almost sure convergence (59), (60) leads to

$$\lim_{\mu_\varepsilon\to 0}\frac{1}{\mu_\varepsilon}\log\mathcal{Z}^\varepsilon(e^h)=\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\prod_{i=1}^{n}f^0\big(\mathbf{z}_i(0)\big)\exp\Big(h\big(\mathbf{z}_i([0,T])\big)\Big), \tag{65}$$

where $\mathbf{Z}_n$ stands for the limiting trajectory as in Definition III.2. Furthemore, the upper bound (62) follows from (63).

To complete the derivation of (61), one has to consider $\mathcal{Z}^\varepsilon(1)$. For $h=0$, the term (65) simplifies as it no longer depends on the precise trajectories and the gain and loss term (in the sums over $s_e=\pm1$) compensate as soon as $n\ge 2$

$$\lim_{\mu_\varepsilon\to 0}\frac{1}{\mu_\varepsilon}\log\mathcal{Z}^\varepsilon(1)=\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\prod_{i=1}^{n}f^0\big(\mathbf{z}_i(0)\big)=\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{z}_1)\;f^0\big(\mathbf{z}_1(0)\big)=\int dz_1\,f^0\big(z_1\big)=1, \tag{66}$$

where we used that f^0 is a probability distribution in the last equality. This proves Proposition III.3. □

B. Derivation of the Boltzmann equation

As a first application of Proposition III.3, we are going to recover Theorem I.1, i.e. that the limiting density of the hard sphere dynamics follows the Boltzmann equation for short times.

We start by introducing a notion of strong solution of the Boltzmann equation (8). For simplicity, we will use a shorthand notation for the collision operator and rewrite (8) as

$$\partial_t f+v\cdot\nabla_x f=\boldsymbol{C}(f,f). \tag{67}$$

By a fix point argument [references], one can show that under the assumptions (5) on f^0 there exists a unique solution of the Boltzmann equation on a time interval $[0,T^\star]$ (assuming here $T^\star > T$ with T defined in Proposition II.3). In particular, this solution is a mild solution and takes the following form for $t \le T^\star$

$$\begin{aligned} f(t) &= \boldsymbol{S}_1(t)f^0 + \int_0^t dt_1 \boldsymbol{S}_1(t-t_1)\boldsymbol{C}\big(f(t_1), f(t_1)\big) \\ &= \boldsymbol{S}_1(t)f^0 + \int_0^t dt_1 \boldsymbol{S}_1(t-t_1)\boldsymbol{C}\,\boldsymbol{S}_2(t_1)f^0\otimes f^0 + \int_0^t dt_1 \int_0^{t_1} dt_2\, \boldsymbol{S}_1(t-t_1)\boldsymbol{C}\,\boldsymbol{S}_2(t_1-t_2)\boldsymbol{C}_2\big(\,(f\otimes f)\,(t_2), f(t_2)\big), \end{aligned}$$

where the operator $\boldsymbol{S}_k(\tau)$ acts as the backward free transport during time τ for k particles. In the second equality, the Duhamel representation has been iterated on each function $f(t_1)$. Another collision may occur at time t_2 on one of the functions $f(t_2)$ and we denote by $\boldsymbol{C}_2$ the corresponding collision operator. We define a *strong solution* of the Boltzmann equation as a solution such that the iteration of Duhamel series is convergent

$$f(t) = \sum_{n=0}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \boldsymbol{S}_1(t-t_1)\boldsymbol{C}\boldsymbol{S}_2(t_1-t_2)\boldsymbol{C}_2 \ldots \boldsymbol{C}_n\boldsymbol{S}_{n+1}(t_n)\left(f^0\right)^{\otimes(n+1)}, \tag{68}$$

where $\boldsymbol{C}_k$ stands for the collision operator applied to one of the k particles in the system. Under the assumptions (5) on the initial data f^0 and by the choice of T, the existence of a strong solution of the Boltzmann equation is well known in $[0,T]$. In fact, this can be deduced as a byproduct of the existence of the solution of the Boltzmann hierarchy, which serves as a limiting structure in the derivation of the Boltzmann equation (see e.g. [GST14]). It is stated in Proposition III.4 as an assumption to stress the fact that, in our approach, the existence of a strong solution of (8) decouples from the rest of the proof.

Proposition III.4 *Let $T>0$ be the convergence time obtained in Proposition II.3. Assuming that there exists a strong solution $\big(f(t)\big)_{t\le T}$ of the Boltzmann equation* (8) *in the time interval $[0,T]$, then the empirical measure converges to the solution of the Boltzmann equation in the following sense : for any $t\le T$, any continuous test function h in $L^\infty(\mathbb{T}^d\times\mathbb{R}^d)$ and $\delta>0$, then*

$$\mathbb{P}_\varepsilon\left(\left|\pi_t^\varepsilon(h) - \int_{\mathbb{T}^d\times\mathbb{R}^d} dz f(t,z)h(z)\right| > \delta\right) \xrightarrow[\mu_\varepsilon\to\infty]{} 0. \tag{69}$$

Note that the controls of the exponential moments in Proposition III.3 can lead to stronger convergence statements than the convergence in probability (69). For example, large deviations estimates were derived in [BGSRS20c].

Proof. To prove Proposition III.4, it is enough to show the convergence in law, i.e. the limit

$$\lim_{\varepsilon\to 0}\mathbb{E}_\varepsilon\left[\pi_t^\varepsilon(h)\right] = \int_{\mathbb{T}^d\times\mathbb{R}^d} dz f(t,z)h(z). \tag{70}$$

Indeed the convergence in probability (69) follows from the Markov inequality and the L^2 inequality

$$\mathbb{E}_\varepsilon\left[\left(\pi_t^\varepsilon(h) - \int dz f(t,z)h(z)\right)^2\right] \le O\left(\frac{\|h\|_\infty^2}{\mu_\varepsilon}\right) + 2\left(\mathbb{E}_\varepsilon\left[\pi_t^\varepsilon(h)\right] - \int_{\mathbb{T}^d\times\mathbb{R}^d} dz f(t,z)h(z)\right)^2, \tag{71}$$

which is a consequence of the concentration estimate (46).

We turn now to the derivation of (70). By Propositions II.3 and III.3, the functionals Λ_T^ε and Λ_T are analytic so that

$$\lim_{\varepsilon\to 0}\mathbb{E}_\varepsilon\left[\pi_{[0,T]}^\varepsilon(h)\right] = \lim_{\varepsilon\to 0}\partial_u\Lambda_T^\varepsilon(e^{uh})\Big|_{u=0} = \partial_u\Lambda_T(e^{uh})\Big|_{u=0}. \tag{72}$$

For a given $t\in[0,T]$, we choose

$$h\big(\mathbf{z}([0,T])\big) = h\big(\mathbf{z}(t)\big),$$

with a continuous test function h in $L^\infty(\mathbb{T}^d\times\mathbb{R}^d)$. Note that the identity (72) is obtained by derivation, so that the condition (14) can be relaxed and it is enough to assume that the test function h belongs to L^∞. Up to now the time window $[0,T]$ was fixed, but it will be convenient to reduce it to $[0,t]$. We deduce, from the identity (72), the limiting counterpart of (43)

$$\begin{aligned} \lim_{\varepsilon\to 0}\mathbb{E}_\varepsilon\left[\pi_t^\varepsilon(h)\right] &= \sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}^{[0,t]}(\mathbf{Z}_n)\left(\sum_{i=1}^n h\big(\mathbf{z}_i(t)\big)\right)\prod_{i=1}^n f^0\big(\mathbf{z}_i(0)\big) \\ &= \sum_{n=1}^{\infty}\frac{1}{(n-1)!}\sum_{\overline{\mathcal{T}}_\prec\in\boldsymbol{\mathcal{T}}_n^{\prec,\pm}}\int d\mu_{\mathrm{sing},\overline{\mathcal{T}}_\prec}^{[0,t]}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big)\prod_{i=1}^n f^0\big(\mathbf{z}_i(0)\big), \end{aligned} \tag{73}$$

the superscript on the measure $\mu^{[0,t]}_{\mathrm{sing},\overline{\mathcal{T}}_\prec}$ indicates that the trajectories are restricted to the time interval $[0,t]$. The second equality is obtained by the symmetry of the particles.

To complete (70), it remains to show that $f(t)$ can be identified as the RHS of (73). For this, we are going to simplify each term of the series (73) by showing that only the particles in a cluster of influence of particle 1 are needed to compute $h\big(\mathbf{z}_1(t)\big)$ (see Figure 5). To extract the relevant information, we consider a signed ordered tree $\overline{\mathcal{T}}_\prec$ of size n and proceed by building recursively a growing collection of trees $\mathcal{A}_1 \subset \mathcal{A}_2 \subset \dots$ as follows. Starting from the vertex $\mathcal{A}_1 = \{1\}$ associated with the particle 1, all the vertices and edges connected to 1 are added to form the set $\mathcal{A}_2$. Suppose that ℓ belongs to $\mathcal{A}_2$ and that the edge $(1,\ell)$ has rank k then all the neighbours of ℓ are added to $\mathcal{A}_3$ provided they are linked to ℓ by an edge with a rank smaller than k, i.e. if the corresponding clustering has occurred before k. Iterating this procedure leads to an ordered tree $\mathcal{A}$ from which the configuration $\mathbf{z}_1(t)$ can be recovered. We will denote by $\boldsymbol{\mathcal{A}}_n^{\prec,\pm}$ the set containing the trees with n vertices of the previous form, i.e. the trees rooted in 1 such that the edge ranks are decreasing when examined from the root to a leaf (see Figure 5).

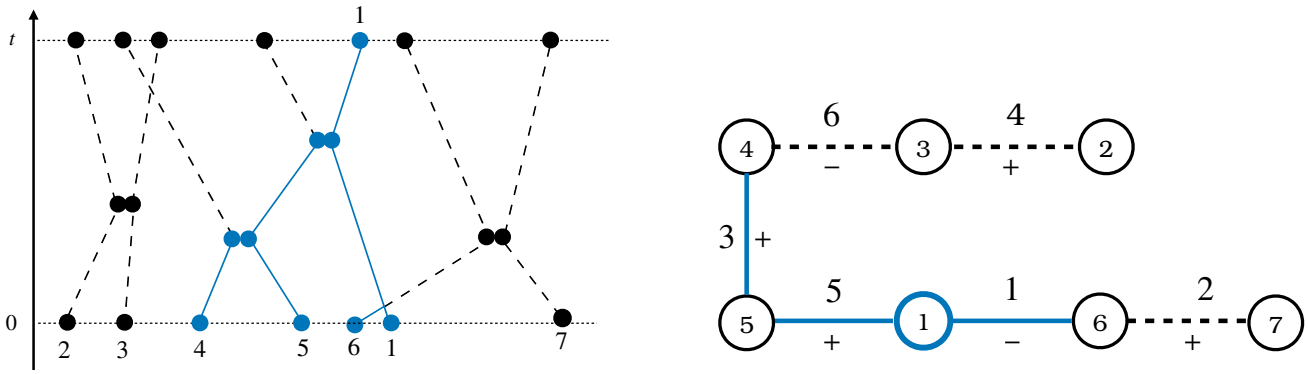

FIG. 5. On the left, particle trajectories associated with a term of order $n = 7$ in (73) are depicted and the corresponding ordered graph $\overline{\mathcal{T}}_\prec$ is depicted on the right : each edge has a rank and a sign $\pm$ to record if it is a collision or an overlap. The relevant part $\mathcal{A}$ of the trajectories, which determine $\mathbf{z}_1(t)$, is represented by blue lines and the edges which can be neglected by dashed lines. Ultimately the initial coordinates of the particles in the blue tree $\mathcal{A}$ and the sign of the clusterings prescribe $\mathbf{z}_1(t)$.

Given $\mathcal{A} \in \boldsymbol{\mathcal{A}}_n^{\prec,\pm}$, let $\overline{\mathcal{T}}_\prec$ be a tree in which $\mathcal{A}$ can be embedded but which has at least one more edge than $\mathcal{A}$. Choosing one leaf in $\overline{\mathcal{T}}_\prec$ which is not in $\mathcal{A}$, one can build another tree $\overline{\mathcal{T}}'_\prec$ by simply changing the sign of the edge connecting this leaf. This changes the tree locally without influencing the value of $h\big(\mathbf{z}_1(t)\big)$ so that

$$\int d\mu^{[0,t]}_{\mathrm{sing},\overline{\mathcal{T}}'_\prec}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big) \prod_{i=1}^{n} f^0\big(\mathbf{z}_i(0)\big) = -\int d\mu^{[0,t]}_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big) \prod_{i=1}^{n} f^0\big(\mathbf{z}_i(0)\big).$$

Thus the sum (73) reduces to

$$\lim_{\varepsilon\to 0} \mathbb{E}_\varepsilon\left[\pi_t^\varepsilon(h)\right] = \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \sum_{\mathcal{A}\in\boldsymbol{\mathcal{A}}_n^{\prec,\pm}} \int d\mu^{[0,t]}_{\mathrm{sing},\mathcal{A}}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big) \prod_{i=1}^{n} f^0\big(\mathbf{z}_i(0)\big).$$

Note that the time ordering of the edges is sufficient to recover from $\mathcal{A}$ the final position $\mathbf{z}_1(t)$. Thus at this stage the labels of the vertices by the $n-1$ other particles in the tree (which is taken into account by the factor $\frac{1}{(n-1)!}$) can be omitted. Denoting by $\hat{\boldsymbol{\mathcal{A}}}_n^{\prec,\pm}$ the set of rooted trees with ordered and signed edges, but without labels on the vertices, we finally obtain

$$\lim_{\varepsilon\to 0} \mathbb{E}_\varepsilon\left[\pi_t^\varepsilon(h)\right] = \sum_{n=1}^{\infty} \sum_{\hat{\mathcal{A}}\in\hat{\boldsymbol{\mathcal{A}}}_n^{\prec,\pm}} \int d\mu^{[0,t]}_{\mathrm{sing},\hat{\mathcal{A}}}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big) \prod_{i=1}^{n} f^0\big(\mathbf{z}_i(0)\big). \tag{74}$$

In the following, we are going to compare this formula with the iterated Duhamel representation of the Boltzmann equation.

We are going to check now that the series (74) coincides with the representation by a Duhamel series (68) of the solution f of the Boltzmann equation. Fixing at time t the position $z = \mathbf{z}_1(t)$ of particle 1, the collision tree $\hat{\mathcal{A}}$ is built backward by adding the particles which are interacting dynamically with particle 1 (cf. Figure 5). The collision operator in (68) leads to the creation of new particles which can be seen as the creation of new edges in the tree $\hat{\mathcal{A}}$. Furthermore, the signed singular measure $\mu^{[0,t]}_{\mathrm{sing},\hat{\mathcal{A}}}$ can be rebuilt thanks to the cross sections in the gain and loss parts of the collision operators. Thus the iterated Duhamel expansion (68) is recovered by following backward the expansion (74). We have therefore proved (70) and completed the derivation of Proposition III.4. □

C. Hamilton-Jacobi equation

The limiting structure derived in Proposition III.3 provides much more informations than the convergence of the particle density to the Boltzmann equation. In particular, it was shown in [BGSRS20c] that the fluctuating Boltzmann equation and the large deviations (quantifying atypical particle evolutions) can be derived from explicit controls on the limit $\Lambda_T(e^h)$ of the exponential moments. These controls were obtained by showing that the limit is related to an Hamilton-Jacobi equation which we state below.

It will be convenient to consider test functions on the trajectories of the form for $t \le T$

$$e^{h(\mathbf{z}^\varepsilon([0,t]))} = \gamma\big(\mathbf{z}^\varepsilon(t)\big)\exp\Big(-\int_0^t \phi\big(s,\mathbf{z}^\varepsilon(s)\big)ds\Big), \tag{75}$$

where $\phi : [0,t]\times\mathbb{T}^d\times\mathbb{R}^d \to \mathbb{C}$ and $\gamma : \mathbb{T}^d\times\mathbb{R}^d \to \mathbb{C}$ are two complex functions defined in the following functional space indexed by the parameters $a \ge 0$ and $\beta > 0$

$$\mathcal{B}_{a,\beta,t} := \Big\{(\phi,\gamma) \in C^0([0,t]\times\mathbb{T}^d\times\mathbb{R}^d;\mathbb{C})\times C^0(\mathbb{T}^d\times\mathbb{R}^d;\mathbb{C}) \;\Big|\; |\gamma(z)| \le e^{(1-\frac{t}{2T})(a+\frac{\beta}{4}|v|^2)}, \quad \sup_{s\in[0,t]}|\phi(s,z)| \le \frac{1}{2T}(a+\frac{\beta}{4}|v|^2)\Big\}.$$

Note that the assumption on h stated in (14) could have been generalised to encompass a (small) quadratic divergence in the velocity as above.

To stress the dependence on ϕ and γ, we rewrite the exponential moment (61) as

$$\forall t \le T, \qquad \mathcal{J}(t,\phi,\gamma) := \Lambda_T\big(\gamma e^{-\int_0^t \phi}\big). \tag{76}$$

Even though Λ_T refers to an expectation on $[0,T]$, it can be restricted to $[0,t]$ as the observables are only in this time range.

The following result was derived in [BGSRS20c].

Theorem III.1 *There are parameters $a,\beta,T > 0$ depending on the initial data f^0 introduced in* (5) *such that the following holds. For all $(\phi,\gamma^\star) \in \mathcal{B}_{a,\beta,T}$, define the function γ in $[0,T]$ by*

$$D_t\gamma_t - \phi_t\gamma_t = 0, \quad \gamma_T = \gamma^\star. \tag{77}$$

Then the functional $\mathcal{J}(t,\phi,\gamma_t)$ satisfies the following Hamilton-Jacobi equation on $[0,T]$:

$$\partial_t\mathcal{J}(t,\phi,\gamma_t) = \frac{1}{2}\int \frac{\delta\mathcal{J}}{\delta\gamma}(t,\phi,\gamma_t)(z_1)\frac{\delta\mathcal{J}}{\delta\gamma}(t,\phi,\gamma_t)(z_2)\Big(\gamma_t(z_1')\gamma_t(z_2') - \gamma_t(z_1)\gamma_t(z_2)\Big)\delta_{x_1-x_2}((v_1-v_2)\cdot\omega)_+ d\omega dv_1 dv_2 dx_1. \tag{78}$$

In an appropriate functional setting, the (local) existence and uniqueness of the solution of the Hamilton-Jacobi equation was also shown in [BGSRS20c]. Thus the Hamilton-Jacobi equation fully characterises the limit of the exponential moments.

The Hamilton-Jacobi equation was derived in [BGSRS20c] by estimating short time increments $\mathcal{J}(t+\delta,\phi,\gamma_{t+\delta}) - \mathcal{J}(t,\phi,\gamma_t)$ thanks to the series expansion stated in Proposition III.3. A similar strategy could have been implemented to recover the Boltzmann equation from the series expansion

$$\int dz f(t,z)h(z) = \sum_{n=1}^\infty \frac{1}{(n-1)!}\sum_{\overline{\mathcal{T}}_\prec \in \boldsymbol{\mathcal{T}}_n^{\prec,\pm}} \int d\mu^{[0,t]}_{\mathrm{sing},\overline{\mathcal{T}}_\prec}(\mathbf{Z}_n)\; h\big(\mathbf{z}_1(t)\big)\prod_{i=1}^n f^0\big(\mathbf{z}_i(0)\big).$$

This method would provide an alternative (but more tedious) derivation of the Boltzmann equation without relying on the direct identification by the iterated Duhamel series as in Section III B.

IV. PERSPECTIVES

The forets play a key role in the cluster expansion of the exponential moment and it would be interesting to study the dynamics of these forests in its own right as a relevant observable of the hard sphere dynamics. This question has already been addressed in [Sin72, Sin74, GKSZ08, PSW16, PSW17, HP19] either from a heuristic point of view or at the level of Kac model in connection with a coalescence process. The methods developed in this paper provide a direct way for studying the particle trajectories and they should allow to prove the convergence, in the Boltzmann-Grad limit, of the forest distribution (in terms of a series related to (61), see [PSW16]) as well as a characterisation of the limiting evolution of a forest which can be described by a Markov process with aggregation rates depending on the law of the process itself (as in Tanaka's process for the Boltzmann equation).

a developper ?

biblio: ordre et labels

[Ale75] Roger Keith Alexander. The infinite hard-sphere system. PhD thesis, University of California, Berkeley, 1975.

[BGSRS18] Thierry Bodineau, Isabelle Gallagher, Laure Saint-Raymond, and Sergio Simonella. One-sided convergence in the Boltzmann–Grad limit. Annales de la Faculté des sciences de Toulouse: Mathématiques, 27(5):985–1022, 2018.

[BGSRS20a] Thierry Bodineau, Isabelle Gallagher, Laure Saint-Raymond, and Sergio Simonella. Fluctuation theory in the Boltzmann–Grad limit. Journal of Statistical Physics, 180(1):873–895, 2020.

[BGSRS20b] Thierry Bodineau, Isabelle Gallagher, Laure Saint-Raymond, and Sergio Simonella. Long-time correlations for a hard-sphere gas at equilibrium. preprint arXiv:2012.03813, to appear in CPAM, 2020.

[BGSRS20c] Thierry Bodineau, Isabelle Gallagher, Laure Saint-Raymond, and Sergio Simonella. Statistical dynamics of a hard sphere gas: fluctuating Boltzmann equation and large deviations. preprint arXiv:2008.10403, 2020.

[BGSRS21] Thierry Bodineau, Isabelle Gallagher, Laure Saint-Raymond, and Sergio Simonella. Large time fluctuations for a hard sphere gas at equilibrium in the low density regime. preprint, 2021.

[Bil99] Patrick Billingsley. Convergence of probability measures. Chichester: Wiley, 1999.

[CGP97] C. Cercignani, V. I. Gerasimenko, and D. Ya. Petrina. Many-particle dynamics and kinetic equations, volume 420 of Mathematics and its Applications. Kluwer Academic Publishers Group, Dordrecht, 1997. Translated from the Russian manuscript by K. Petrina and V. Gredzhuk.

[CIP94] Carlo Cercignani, Reinhard Illner, and Mario Pulvirenti. The mathematical theory of dilute gases, volume 106 of Applied Mathematical Sciences. Springer-Verlag, New York, 1994.

[Den18] Ryan Denlinger. The propagation of chaos for a rarefied gas of hard spheres in the whole space. Arch. Ration. Mech. Anal., 229(2):885–952, 2018.

[FV17] Sacha Friedli and Yvan Velenik. Statistical mechanics of lattice systems: a concrete mathematical introduction. Cambridge University Press, 2017.

[GG18] Viktor Gerasimenko and Igor Gapyak. Low-density asymptotic behavior of observables of hard sphere fluids. Adv. Math. Phys., 2018:11, 2018.

[GG21] V. I. Gerasimenko and I. V. Gapyak. Boltzmann-Grad asymptotic behavior of collisional dynamics. Rev. Math. Phys., 33(2):32, 2021.

[GKSZ08] A. Gabrielov, V. Keilis-Borok, Ya. Sinai, and I. Zaliapin. Statistical properties of the cluster dynamics of the systems of statistical mechanics. In Boltzmann's legacy. Papers based on the presentations at the international symposium, Vienna, Austria, June 7–9, 2006., pages 203–215. Zürich: European Mathematical Society (EMS), 2008.

[Gra49] Harold Grad. On the kinetic theory of rarefied gases. Commun. Pure Appl. Math., 2:331–407, 1949.

[GST14] Isabelle Gallagher, Laure Saint-Raymond, and Benjamin Texier. From Newton to Boltzmann: hard spheres and short-range potentials. Zürich: European Mathematical Society (EMS), 2014.

[HP19] Daniel Heydecker and Robert IA Patterson. Bilinear coagulation equations. preprint arXiv:1902.07686, 2019.

[IP89] R. Illner and M. Pulvirenti. Global validity of the Boltzmann equation for two-and three-dimensional rare gas in vacuum: Erratum and improved result. Commun. Math. Phys., 121(1):143–146, 1989.

[Lan75] Oscar E. Lanford, III. Time evolution of large classical systems, pages 1–111. Lecture Notes in Phys., Vol. 38. 1975.

[MT12] Karsten Matthies and Florian Theil. A semigroup approach to the justification of kinetic theory. SIAM J. Math. Anal., 44(6):4345–4379, 2012.

[Pen67] Oliver Penrose. Convergence of fugacity expansions for classical systems. page 101. Benjamin, New York, 1967.

[PS17] 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.

[PSS14] M. Pulvirenti, C. Saffirio, and S. Simonella. On the validity of the Boltzmann equation for short range potentials. Rev. Math. Phys., 26(2):1450001, 64, 2014.

[PSW16] Robert I. A. Patterson, Sergio Simonella, and Wolfgang Wagner. Kinetic theory of cluster dynamics. Phys. D: Nonlin. Phen., 335:26–32, 2016.

[PSW17] Robert I. A. Patterson, Sergio Simonella, and Wolfgang Wagner. A kinetic equation for the distribution of interaction clusters in rarefied gases. J. Stat. Phys., 169(1):126–167, 2017.

[PU09] Suren Poghosyan and Daniel Ueltschi. Abstract cluster expansion with applications to statistical mechanical systems. Journal of mathematical physics, 50(5):053509, 2009.

[Rue99] David Ruelle. Statistical mechanics. World Scientific Publishing Co., Inc., River Edge, NJ; Imperial College Press, London, 1999. Rigorous results, Reprint of the 1989 edition.

[Sim14] Sergio Simonella. Evolution of correlation functions in the hard sphere dynamics. J. Stat. Phys., 155(6):1191–1221, 2014.

[Sin72] Ja. G. Sinaĭ. Construction of the dynamics for one-dimensional systems of statistical mechanics. Teoret. Mat. Fiz., 11(2):248–258, 1972.

[Sin74] Ja. G. Sinaĭ. Construction of a cluster dynamic for the dynamical systems of statistical mechanics. Vestnik Moskov. Univ. Ser. I Mat. Meh., 29(1):152–158, 1974. Collection of articles dedicated to the memory of Ivan Georgievič Petrovskiĭ.

[Spo81] Herbert Spohn. Fluctuations around the Boltzmann equation. J. Statist. Phys., 26(2):285–305, 1981.

[Spo12] Herbert Spohn. Large scale dynamics of interacting particles. Springer Science & Business Media, 2012.

[Uel04] Daniel Ueltschi. Cluster expansions and correlation functions. Moscow Math. J., 4:511–522, 2004.