PACKET DECOMPOSITION OF HARD SPHERE DYNAMICS

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Abstract. We identify a natural dynamical object, packet, in hard sphere systems. Then we apply the cluster expansion to calculate the partition function and find a new proof of convergence in the low-density Boltzmann-Grad limit. As an application, we use this packet method to derive the Hamilton-Jacobi equation satisfied by the partition function.

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1. Introduction

In this mémoire, we will study collisions in a large system of hard-core particles following deterministic Newton's law, in a low-density limit. We will briefly introduce our system of interest, recall a classical result, and descibe our new approach to recover the result.

1.1. **Interacting particle systems.**

It is hard to imagine different types of matter, gas, liquid and solid, which constitute our world, are formed by microscopic molecules following the same physical law. More surprisingly, the same group of molecules under different conditions can appear drastically different. The origin of such phenomenon is the interaction between particles, without which the only type of matter would be ideal gas.

There are many possible interactions. For example, or neutral molecules, their interaction can be describe by Lennard-Jones potential:

$$V_{\mathrm{LR}}\left(r\right)=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right],$$

and for charged particles, the electrical potential apply

$$V_{\mathrm{E}}\left(r\right)=\frac{1}{4\pi\varepsilon_0}\frac{1}{r}.$$

However, we will not study these more realistic interactions, instead we will only consider the idealized model of hard spheres. These are particles with a defined radius and whose boundary is infinitely hard. Particles move freely with constant velocity, until some of them collide with each other. The collision is assumed to be completely elastic with no friction, conserving energy and exchanging only momentum along the axe of collision (line connecting the center of particles). The reason for studying this system is because of its simplicity, and one can even argue that this is the simplest interaction among all. This interaction, different from Lennard-Jones and electrical, is of compact support, meaning that particles' trajectory will not be deflected at all when they are spatially distant from each other. This allows us to focus on the relatively rare event when particles collide, since for the rest of time they simply move in straight line.

Once the interaction is specified, one can apply Newton's law to predict the motion of particles, and calculate the macroscopic quantities, for example, particle density and pressure. This approach is not only computationally infeasible, but also lacks the information of the initial condition to start with. Moreover, possible chaotic phenomena destroy the hope of finding an approximative solution, if the converse is not proved.

We will not try to find a precise initial condition which happens to describe a system of particles in a lab. Instead, we add a layer of randomness to the initial condition by specifying a probability measure on the phase space, admitting that the information we have is incomplete. We then let the particle system with different initial conditons to evovle deterministically.

Suppose we have a macroscopic (density) distribution function of the particles $f^0\left(x,v\right)$, conventionally normalized so that $\int dxdvf^0\left(x,v\right)=1$. This distribution function indicates that the number of particles with position in $[x,x+dx]$, velocity in $[v,v+dv]$ is propotional to

$$f^0\left(x,v\right)dxdv.$$

Although there are many other candidates who can reproduce this particle density distribution, we will choose a measure which to close to the product measure, to maximize the independence between different particles. Moreover, instead of fixing the number of particles, we will let the number of particles follows Poisson law very close, again to maximize the independence.

We refer to [6] for a review of different interacting particle systems with deterministic and stochastic dynamics.

1.2. **Boltzmann-Grad limit and Lanford's theorem.** In 1975 Lanford proved in his seminal work [5] that the distribution function of the hard sphere system, in a low density limit, converges to the solution f of the Boltzmann equation for a short time:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = C\left(f, f\right).$$

Moreover, the N-particle correlation factorizes into a product of single particle correlation function in the limit. For our case of variable particle number, we refer to [4].

With Lanford's theorem, one can make predictions about a very large system by only calculating macroscopic distribution functions. The factorization of distribution function implies independence between particles, which allows us to derive a law of large number for the hard spheres dynamics (Section 1.2, [2]).

The limiting procedure is done by fixing a volume, letting the particle size go to zero and the number of particles go to infinity. To be precise, suppose the spatial dimension is d, the diameter of the hard sphere is ε and the number of particles is N, we will consider the dynamics in $\mathbb{T}^d$, the d-dimensional torus. We will keep

$$N\varepsilon^{d-1} = 1$$

and let $\varepsilon \to 0$. This is called the *Boltzmann-Grad* limit. Note that in this limit the density of particles, which is the spatial volume occupied by particles per unit volume, decreases to 0, while in the usual physical thermodynamical limit this quantity is kept constant. One could speculate that Boltzmann equation could only be a good approximation of real-world system of very low density.

Although the density is not fixed, in Lanford's setting, the *mean free path* of particles is stable. The mean free path is the average distance between two consecutive collisions a particle enters in. In fact, we can pick a tagged particle, and work in the frame moving along with the particle. From 0 until time t, the trajectory of the i-th particle will occupy a space volume $C_d\varepsilon^{d-1}v_{\mathrm{rel},i}t$ and it will collide with the tagged one if and only if the origin of coordinate system is contained in this space volume. Summing up for all i, the probability of having at least one collision before time t is approximatively

$$C_dN\varepsilon^{d-1}v_{\mathrm{rel},i}t.$$

By integrating the initial velocities, the quantity becomes propotional to

$$C_dN\varepsilon^{d-1}t.$$

Since $N\varepsilon^{d-1}$ is kept constant, the probability of entering into collisions is stable during the limit. Therefore the mean free path is stable.

1.3. **Packets, partition function, cluster expansion.** Instead of studying the individual particles, we will study the hard sphere dynamics by investigating the groups of particles whose dynamics become interdependent because of collisions. We will call such groups *packets*. By the nature of the hard-core interaction, the dynamics of different packets are very weakly correlated—they are independent of each other as long as particles in different packets do not collide.

Luckily, in statistical physics we have already the tool for studying such weakly interacting system—*cluster expansion*. In the statistical physics context, the quantity of interest is the *partition function* of the system, which is a weighted sum of all system configurations. Suppose, for example, our system have N particles living on $\mathbb{R}$, interacting through a two-body potential $u(r)$. Let $d\mu$ be the probability measure of a free particle, i.e. one which does not interact at all. Then the partition function defined as

$$\mathcal{Z} = \int \prod_{i=1}^{N} d\mu\left(x_i\right) \exp\left(-\beta \sum_{1\le i<j\le N} u\left(x_i - x_j\right)\right).$$

Now in the cluster expansion approach we suppose furthermore that the interaction $u(r)$ is weak, so that $u \approx 0$, or $\exp u \approx 1$. Define

$$\exp\left(-\beta u\left(x_i - x_j\right)\right) = 1 + f_{ij}.$$

The interaction term can be expanded

$$\begin{aligned} \text{(1)} \quad \exp\left(-\beta \sum_{1\le i<j\le N} u\left(x_i - x_j\right)\right) &= \prod_{1\le i<j\le N} \left(1 + f_{ij}\right) \\ &= 1 + \sum_{1\le i<j\le N} f_{ij} + \sum_{1\le i<j\le N} \sum_{1\le k<l\le N} \mathbf{1}_{\{i,j\}\neq\{k,l\}} f_{ij} f_{kl} + \cdots \end{aligned}$$

where the expansion can be think as power series in the strength of interaction.

Physicists have calculate the partition function of numerous systems with this approach. We, however, will use a theorem of [7] to obtain an expression of $\log \mathcal{Z}$. It is natural to consider logarithm, since for non-interacting system we will have $\mathcal{Z} = \mathcal{Z}^N_{\text{single particle}}$, so $\log \mathcal{Z}$ will be expected to scale linearly with the number of particles in the system. More importantly, after taking log, the weak interaction between different packets becomes a strong connectivity constraint on the relative position of the packets.

For a more physical introduction to the cluster expansion approach, we refer to [3].

1.4. **Organization of the mémoire.** We first formally define the hard sphere dynamics and introduce a probability measure on initial condition. Then we define packets formally and rewrite the partition function in terms of packets. After applying cluster expansion to the packet representation, we find that the domain of integration is on some rare events where particles and packets become connected in a sense. We change to another set of parameters to suit better these events. Using two technical lemmas, we could clean the clutter in our integration of partition function and prove the convergence to a limiting integration scheme. As an application, we derive the Hamilton-Jacobi equation satisfied by the partition function by using the limiting integration scheme and exploiting some independence between packets.

Finally, we show that Boltzmann equation is nothing but the first-order term of Hamilton-Jacobi.

2. Hard sphere dynamics

We will study the dynamics of a groups of Newtonian *hard-sphere* particles, the simplest system of interacting particles. In a general Newtonian setting, we will indicate the initial condition of the system, i.e. the initial position and velocity of particles, and also specify the interaction by introducing a two-body potential $V:\mathbb{R}^3\to\mathbb{R}$. Suppose there are a fixed number, N, of particles. Let x_i, v_i be the time-dependent position and velocity of the i-th particle. According to the second law of Newton, the dynamics is determined by the following ordinary differential equations (ODEs).

$$\begin{aligned}\frac{dx_i}{dt} &= v_i,\\ \frac{dv_i}{dt} &= -\sum_{j\neq i}\nabla V\left(x_i-x_j\right).\end{aligned}$$

We need to assume the differentiablity of V to make sense of the equations. Further conditions are necessary to ensure the existence and uniqueness of solutions.

The system of interest, however, departs from the general setting since the interaction potential will be result of a limiting process, which inevitably becomes singular. We will not discuss the limiting process since this adds extra technicality, and will not be useful in the rest of paper. Instead, we define the system without ODEs, and state a result of existence and uniqueness, similar to that of solutions of ODEs.

We fix d to be the spatially dimension of systems of interest throughout the paper. We will consider only systems with periodical boundary conditions, i.e. the particles move in a d-dimensional torus $\mathbb{T}^d$. We will also use $\mathbb{D}:=\mathbb{T}^d\times\mathbb{R}^d$ to denote the single-particle phase space.

Definition 1 (Hard-sphere dynamics with periodic boundary conditions)**.** Let N be the number of particles and ε be the size of particles, and $Z^N=(x_i,v_i)_{i=1}^N\in\mathbb{D}_\varepsilon^N$ where

$$\mathbb{D}_\varepsilon^N:=\left\{(x_i,v_i)_{i=1}^N\in\left(\mathbb{T}^d\times\mathbb{R}^d\right)^N:\forall i\neq j,|x_i-x_j|>\varepsilon\right\}.$$

We will call Z^N the initial condition of the hard-sphere dynamics, respectively. Set the present time $t_{\mathrm{c}}=0$ and $x_i(0)=x_i$, $v_i(0)=v_i$. The dynamics is defined in the following iterative way:

(1) For time $t\geq t_{\mathrm{c}}$, let $x_i(t)=x_i(t_p)+v_i(t_p)(t-t_p)$, $v_i(t)=v_i(t_p)$, until
(2) a time $t_{\mathrm{c,new}}$ when the distance of two particles becomes equal or smaller than ε, i.e.

$$t_{\mathrm{c,new}}=\inf\left\{t>t_{\mathrm{c}}:\exists i<j,|x_i(t)-x_j(t)|\leq\varepsilon\right\}.$$

We will say such particles i,j *collide* at time $t_{\mathrm{c,new}}$. If there exist multiple pairs of $i<j$ colliding at time $t_{\mathrm{c,new}}$, the dynamics is not defined. In the case where there exists only one pair $i<j$, let $\omega=\varepsilon^{-1}(x_j-x_i)$. We

modify the velocities as follows

$$v_i(t_{\mathrm{c,new}}) = v_i(t_{\mathrm{c,new}}-) - [(v_i(t_{\mathrm{c,new}}-) - v_j(t_{\mathrm{c,new}}-)) \cdot \omega]\,\omega,$$
$$v_j(t_{\mathrm{c,new}}) = v_j(t_{\mathrm{c,new}}-) + [(v_i(t_{\mathrm{c,new}}-) - v_j(t_{\mathrm{c,new}}-)) \cdot \omega]\,\omega,$$

set $t_{\mathrm{c}} = t_{\mathrm{c,new}}$, and go back to (1).

The dynamics will not be defined in all $t > 0$ if in one iteration we have $t_{\mathrm{c,new}} = t_{\mathrm{c}}$.

Remark. There are physical acceptable cases which are not defined in the sense of definition , for example the case where two spatially distant collisions happen at exactly the same time. However, we can ignore such cases since they are negligible, which will be clarified in the following.

Theorem 1 (Proposition 2.1 of [1]). *Follow the notation of Definition 2. Equip $\mathbb{D}_\varepsilon^N$ with the Lebesgue measure inherited from $\left(\mathbb{T}^d \times \mathbb{R}^d\right)^N$. Then the hard-sphere dynamics is defined for all positive time for almost all initial conditions on $\mathbb{D}_\varepsilon^N$.*

Remark. We can remove a negligible part from $\mathbb{D}_\varepsilon^N$ such that the hard-sphere dynamics can be considered as a one-parameter group of measure-preserving on the rest.

From now on we will introduce some randomness to the hard sphere dynamical system, by giving a probability measure on the initial condition. Note that the dynamics, once given initial condition, is completely deterministic.

Definition 2. Let $f^0 : \mathbb{D} \to \mathbb{R}$ be a probability distribution function satisfying the following bound

$$\left|f^0(x,v)\right| + \left|\nabla_x f(x,v)\right| \le C_0 \beta_0^{\frac{d}{2}} \exp\left(-\frac{\beta_0 v^2}{2}\right), \quad C_0 > 0, \beta_0 > 0.$$

We may construct a probability measure $\mathbb{P}_\varepsilon$ on space

$$\mathbb{P} := \coprod_{i=0}^{\infty} \mathbb{D}^n$$

by specifying its restriction on each disjoint component, i.e. $\mathbb{P}_\varepsilon|_{\mathbb{D}^n}$. For our purpose, we will choose

$$d\,\mathbb{P}_\varepsilon|_{\mathbb{D}^n} = \frac{1}{\mathcal{Z}^\varepsilon} \frac{\mu_\varepsilon^n}{n!} dz_1 \cdots dz_n f^0(z_1) \cdots f^0(z_n)\, \mathbf{1}_{\mathbb{D}_\varepsilon^n}$$

where $\mu_\varepsilon := \varepsilon^{-(d-1)}$ and $\mathcal{Z}^\varepsilon$ is the normalization factor defined by

$$\mathcal{Z}^\varepsilon := \sum_{n=0}^{\infty} \frac{\mu_\varepsilon^n}{n!} \int_{\mathbb{D}_\varepsilon^n} dz_1 \cdots dz_n \prod_{k=1}^{n} f^0(z_k).$$

We will use $\mathbb{E}_\varepsilon[\cdot]$ to denote expection with respect to this measure.

Remark. Note that if there were no exclusion of particles, i.e. we no longer demand $(z_1, \dots, z_n) \in \mathbb{D}_\varepsilon^n$, the measure would become Poissonian of density $\mu_\varepsilon f^0$. We introduce this measure to ensure the particles are as independent from each other as possible.

We will also fix f^0 (and correspondingly C_0, β_0) throughout the paper.

3. Cluster expansion

In this section, we define packets in hard-sphere dynamics and use these objects to represent the (biased) partition function. This representation introduces hard-core type interaction between different packets, which yields a simple cluster expansion.

3.1. **Defining packets and rewriting the partition function.**

From now on we fix a finite time $t > 0$ and particle size $\varepsilon > 0$. Let $h : \mathbb{D} \to \mathbb{R}$ be a smooth enough function (which will be specified later) on the single-particle phase space.

Let $1 \leq i, j \leq \mathcal{N}$ be two particles in the hard-sphere dynamics. We write $i \sim j$ *(or particles i, j are connected by collision)* if the two particles collide in time interval $[0, t]$. In the contrary case, we write $i \not\sim j$

Definition 3. A subset $P \subset \{1, \dots, \mathcal{N}\}$ is called *connected by collisions* if for any two particles i, j in P, they are either connected, or there exists a sequence of particles $\{k_1, \dots, k_m\} \subset S$ such that $i \sim k_1, k_1 \sim k_2, \dots, k_{m-1} \sim k_m, k_m \sim j$.

We denote by X_P the indication function of this event.

Definition 4. Two subsets $P_1, P_2 \subset \{1, \dots, \mathcal{N}\}$ are called *connected by collisions* if there exists $i \in P_1, j \in P_2$ such that i, j are connected.

By an abuse of notation, we denote this event by $P_1 \sim P_2$. We denote the contrary case by $P_1 \not\sim P_2$.

In the case when the dynamics of P_1, P_2 are mutually independent, we also say P_1, P_2 *overlap* if $P_1 \sim P_2$.

Definition 5. A subset $P \subset \{1, \dots, \mathcal{N}\}$ is called a *packet* if both of the followings are satisfied:

- P is connected by collision.
- P is not connected by collision with $P^c := \{1, \dots, \mathcal{N}\} \setminus P$.

In other words, packets are equivalence classes of the equivalence relation generated by connectivity by collision.

The dynamics of packets is simple. Different packets do not interact, as long as they do not collide with each other, which resembles the behaviour of individual particles.

Definition 6. Let h be a bounded function, we define

$$\begin{aligned}
\mathcal{Z}^{t,\varepsilon}(h) &:= \sum_{n \geq 0} \frac{\mu_\varepsilon^n}{n!} \int dz_1 f^0(z_1) \cdots dz_n f^0(z_n) \prod_{i=1}^{n} \exp h\left(\mathbf{z}_i^\varepsilon(t)\right) \prod_{1 \leq i_1, i_2 \leq n} \mathbf{1}_{|z_{i_1} - z_{i_2}| > \varepsilon} \\
&= \mathcal{Z}^\varepsilon \, \mathbb{E}_\varepsilon \left[\exp \sum_{i=1}^{\mathcal{N}} h\left(\mathbf{z}_i^\varepsilon(t)\right) \right].
\end{aligned}$$

and call it *biased partition function*, or *exponential moment.*

Denote $\mathcal{P}_n^l$ the set of partition of $\{1, \dots, n\}$ into l parts. Let $\lambda \in \mathcal{P}_n^l$ be such a partition, conventionally we set $\lambda = \{\lambda_1, \dots, \lambda_l\}$ (which is an unordered list). We now decompose the unity as follows.

$$\begin{aligned}\mathbf{1}_{\{\mathcal{N}=n\}} &= \mathbf{1}_{\{\mathcal{N}=n\}} \sum_{l=1}^{n} \sum_{\lambda\in\mathcal{P}_n^l} \mathbf{1}_{\{\text{particles form packets } \{\lambda_1,\dots,\lambda_l\}\}} \\ &= \mathbf{1}_{\{\mathcal{N}=n\}} \sum_{l=1}^{n} \sum_{\lambda\in\mathcal{P}_n^l} \prod_{j=1}^{l} X_{\lambda_j} \prod_{1\le j_1<j_2\le l} \left(1-\mathbf{1}_{\left\{\lambda_{j_1}\sim\lambda_{j_2}\right\}}\right).\end{aligned}$$

We recall that the term X_{λ_j} stands for the connectivity by collision inside a packet, defined in Definition 3.

Next, we rewrite the initial condition of mutual exclusion between the particles in terms of condition imposed on $\lambda = \{\lambda_1, \dots, \lambda_l\}$.

$$\begin{aligned}&\mathbf{1}_{\{\mathcal{N}=n\}} \prod_{1\le i_1,i_2\le n} \mathbf{1}_{\left|z_{i_1}-z_{i_2}\right|>\varepsilon} \\ =&\mathbf{1}_{\{\mathcal{N}=n\}} \sum_{l=1}^{n} \sum_{\lambda\in\mathcal{P}_n^l} \mathbf{1}_{\left|z_{i_1}-z_{i_2}\right|>\varepsilon} \prod_{j=1}^{l} X_{\lambda_j} \prod_{1\le j_1<j_2\le l} \left(1-\mathbf{1}_{\left\{\lambda_{j_1}\sim\lambda_{j_2}\right\}}\right) \\ =&\mathbf{1}_{\{\mathcal{N}=n\}} \sum_{l=1}^{n} \sum_{\lambda\in\mathcal{P}_n^l} \prod_{j=1}^{l} \left(X_{\lambda_j}\mathbf{1}_{\{\text{particles in } \lambda_j \text{ do not overlap initially}\}}\right)\cdots \\ &\cdots \prod_{1\le j_1<j_2\le l} \left(1-\mathbf{1}_{\left\{\lambda_{j_1}\sim\lambda_{j_2}\right\}}\right).\end{aligned}$$

Note that if $\lambda_{j_1}, \lambda_{j_2}$ are different packets, the *initial* exclusion between particles in respective subsets

$$\prod_{i_1\in\lambda_{j_1},i_2\in\lambda_{j_2}} \mathbf{1}_{\left|z_{i_1}-z_{i_2}\right|>\varepsilon}$$

are already included in the *dynamical* exclusion of different packets

$$\prod_{1\le j_1<j_2\le l} \left(1-\mathbf{1}_{\left\{\lambda_{j_1}\sim\lambda_{j_2}\right\}}\right).$$

For notational convenience, we let (IE for *Initial Exclusion*)

$$\mathbf{1}_{\{\text{particles in } \lambda_j \text{ do not overlap initially}\}} =: \mathrm{IE}_{\lambda_j}.$$

Using this packet decomposition, we can re-express the partition function as

$$\begin{aligned}\mathcal{Z}^{t,\varepsilon}(h) = \sum_{n\ge 0}\sum_{l=1}^{n}\sum_{\lambda\in\mathcal{P}_n^l} \frac{\mu_\varepsilon^n}{n!} \int \prod_{j=1}^{l} \left(\prod_{i\in\lambda_j} \left(dz_i f^0(z_i) \exp h\left(\mathbf{z}_i^\varepsilon(t)\right)\right) \mathrm{IE}_{\lambda_j} X_{\lambda_j}\right) \\ \cdot \prod_{1\le j_1<j_2\le l} \left(1-\mathbf{1}_{\left\{\lambda_{j_1}\sim\lambda_{j_2}\right\}}\right).\end{aligned} \tag{2}$$

In case when two distinct packets become connected by a collision, the dynamics become not defined after the collision. However, we can extend the definition of dynamics by letting the particles in these packets to continue moving in space, only colliding with particles within the same packet. This will not change any computation result, since extending function on a set of measure zero will not change the integration of the function. In these cases, the trajectories of two packets cross without deflection. We will call such phenomena *overlappings*.

The integration and interaction between particles have been transformed into these of packets, and we define the following

Definition 7 (Packet measure)**.** For $m \geq 1, t > 0, \varepsilon > 0$ and $v_1, \ldots, v_m \in \mathbb{R}^d$, the *$m$-packet measure* is a measure on the m-particle phase space $\mathbb{D}^m$, defined as follows

$$dM_*^{t,\varepsilon,m}\left(x_1, \ldots, x_m\right) = \frac{\mu_\varepsilon^{m-1}}{m!} \bigotimes_{i=1}^{m} dx_i \mathrm{IE}_{\{x_1,\ldots,x_m\}} X_{\{z_1,\ldots,z_m\}}. \tag{3}$$

Note that the dependency on initial velocities is introduced by $X_{\{z_1,\ldots,z_m\}}$, and not explicitly expressed in the notation $dM_*^{t,\varepsilon,m}$. Moreover, the base measure $\otimes_{i=1}^m \mu$ and the conditions $\mathrm{IE}_{\{z_1,\ldots,z_m\}}, X_{\{z_1,\ldots,z_m\}}$ are all translation-invariant. We can further decompose the packet measure by selecting a distinguished particle (for example 1) and expressing all the measures and conditions in terms of relative distances $x_2 - x_1, \ldots, x_m - x_1$ and absolute velocities $v_1, \ldots, v_m$. In other words, there exists a *reduced m-packet measure* $M^{t,\varepsilon,m}$ such that

$$dM_*^{t,\varepsilon,m}\left(z_1, \ldots, z_m\right) = dx_1 \otimes dM^{t,\varepsilon,m}\left(x_2 - x_1, \ldots, x_m - x_1, v_1, \ldots, v_m\right). \tag{4}$$

As a convention, we will use $x_{\lambda_j}^1$ to denote the initial position of the distinguished particle in λ_j.

Remark. As we will see in Proposition 3, the connectivity condition imposes strong constraints on the particles' configuration in a packet, which compensates the factor μ_ε^{m-1} in the front.

We will use $\int dv_{\lambda_j}$ to denote integration of initial velocity of particles in λ_j. The expression for biased partition function can be slightly simplified:

$$\begin{aligned}\mathcal{Z}^{t,\varepsilon}\left(h\right) = &\sum_{n\geq 0} \sum_{l=1}^{n} \sum_{\lambda \in \mathcal{P}_n^l} \mu_\varepsilon^l \frac{|\lambda_1|! \cdots |\lambda_l|!}{n!} \\ &\cdot \int \prod_{j=1}^{l} \left(dv_{\lambda_j} dx_{\lambda_j}^1 dM^{t,\varepsilon,|\lambda_j|} \exp \sum_{i\in\lambda_j} h\left(\mathbf{z}_i^\varepsilon\left(t\right)\right) \prod_{i\in\lambda_j} f^0\left(z_i\right) \right) \\ &\qquad \cdot \prod_{1\leq j_1<j_2\leq l} \left(1 - \mathbf{1}_{\{\lambda_{j_1}\sim\lambda_{j_2}\}}\right).\end{aligned}$$

Here we used the shorthand notation z_{λ_j} to stand for initial position and velocity of all particles in λ_j.

Note that what follows the summation $\sum_{\lambda\in\mathcal{P}_n^l}$ depends only on the size of the partition, i.e. the unordered list $\{|\lambda_1|, \ldots, |\lambda_1|\}$, we can therefore replace the summation by the numerical one

$$\sum_{\substack{m_1+\cdots+m_l=n \\ m_1,\ldots,m_l\geq 1}} \frac{n!}{l! m_1! \cdots m_l!}.$$

Thus,

$$\mathcal{Z}^{t,\varepsilon}(h) = \sum_{n\geq 0}\sum_{l=1}^{n}\sum_{\substack{m_1+\cdots+m_l=n\\ m_1,\ldots,m_l\geq 1}}\frac{\mu_\varepsilon^l}{l!}$$
$$\cdot\int\prod_{j=1}^{l}\left(dv_{\lambda_j}dx^1_{\lambda_j}dM^{t,\varepsilon,|\lambda_j|}\exp\sum_{i\in\lambda_j}h\left(\mathbf{z}_i^\varepsilon(t)\right)\prod_{i\in\lambda_j}f^0(z_i)\right)$$
$$\cdot\prod_{1\leq j_1<j_2\leq l}\left(1-\mathbf{1}_{\{\lambda_{j_1}\sim\lambda_{j_2}\}}\right).$$

Here one should understand $\lambda_1,\ldots,\lambda_l$ as disjoint sets of indices, of size $m_1,\ldots,m_l$ respectively.

By interchanging the order of summations,

$$\begin{aligned}\mathcal{Z}^{t,\varepsilon}(h) &= \sum_{n\geq 0}\sum_{l=1}^{n}\sum_{\substack{m_1+\cdots+m_l=n\\ m_1,\ldots,m_l\geq 1}}\frac{\mu_\varepsilon^l}{l!}\\
&\quad\cdot\int\prod_{k=1}^{l}\left(dv_{\lambda_j}dx^1_{\lambda_j}dM^{t,\varepsilon,|\lambda_j|}\exp\sum_{i\in\lambda_j}h\left(\mathbf{z}_i^\varepsilon(t)\right)\prod_{i\in\lambda_j}f^0(z_i)\right)\\
&\quad\cdot\prod_{1\leq j_1<j_2\leq l}\left(1-\mathbf{1}_{\{\lambda_{j_1}\sim\lambda_{j_2}\}}\right)\\
&= 1+\sum_{l=1}^{\infty}\frac{\mu_\varepsilon^l}{l!}\sum_{m_1,\ldots,m_l\geq 1}\\
&\quad\cdot\int\prod_{k=1}^{l}\left(dv_{\lambda_j}dx^1_{\lambda_j}dM^{t,\varepsilon,|\lambda_j|}\exp\sum_{i\in\lambda_j}h\left(\mathbf{z}_i^\varepsilon(t)\right)\prod_{i\in\lambda_j}f^0(z_i)\right)\\
&\quad\cdot\prod_{1\leq j_1<j_2\leq l}\left(1-\mathbf{1}_{\{\lambda_{j_1}\sim\lambda_{j_2}\}}\right).\end{aligned}$$

Note that this expression of the partition function implies that the hard-sphere dynamics is equivalent to a grand-canonical ensemble of packets with hard-core type interaction.

3.2. **Simplifying packet interaction by cluster expansion.** In this subsection we employ a theorem of Ueltschi to perform the cluster expansion. Using this expansion, we obtain an expression for the logarithm of the biased partition function, moreover, the interaction between packets is simplified.

Let $(\mathbb{A},\mathcal{A},\mu)$ be a measure space; μ is a complex measure and $|\mu|(\mathbb{A})<\infty$, where $|\mu|$ is the total variation (absolute value) of μ. Let ζ be a complex measurable symmetric function on $\mathbb{A}\times\mathbb{A}$.

We denote by $\mathcal{G}_n$ the set of all (unoriented) graphs with n vertices, and $\mathcal{C}_n\subset\mathcal{G}_n$ the set of connected graphs of n vertices. We introduce the following combinatorial function on finite sequences $(A_1,\ldots,A_n)$ of $\mathbb{A}$:

$$\varphi(A_1,\ldots,A_n)=\begin{cases}1 & \text{if } n=1\\ \frac{1}{n!}\sum_{G\in\mathcal{C}_n}\prod_{(i,j)\in G}\zeta(A_i,A_j) & \text{if } n\geq 2.\end{cases}\tag{5}$$

The product is over edges of G. A sequence $(A_1, \dots, A_n)$ is a *cluster* if the graph with n vertices and an edge between i and j whenever $\zeta(A_i, A_j) \neq 0$, is connected.

We recall the following theorem of Ueltschi [7].

Theorem 2 (Cluster expansion)**.** *Assume that* $|1+\zeta(A, A')| \leq 1$ *for all* $A, A' \in \mathbb{A}$, *and that there exists a nonnegative function* a *on* $\mathbb{A}$ *such that for all* $A \in \mathbb{A}$,

$$\int d|\mu|(A')\, |\zeta(A, A')|\, e^{a(A')} \leq a(A), \tag{6}$$

and $\int d|\mu|(A) e^{a(A)} < \infty$. *Then we have*

$$Z = \exp\Big\{\sum_{n\geq 1} \int d\mu(A_1) \dots d\mu(A_n)\, \varphi(A_1, \dots, A_n)\Big\}.$$

Combined sum and integrals converge absolutely. Furthermore, we have for all $A_1 \in \mathbb{A}$

$$1 + \sum_{n\geq 2} n \int d|\mu|(A_2) \dots d|\mu|(A_n)\, |\varphi(A_1, \dots, A_n)| \leq e^{a(A_1)}. \tag{7}$$

We will apply this theorem to the packet measure space $\left(\mathbb{P}, M^{t,\varepsilon,h}\right)$ and the cluster expansion interaction $\left(z_{\lambda_{j_1}}, z_{\lambda_{j_2}}\right) \mapsto -\mathbf{1}_{\left\{\lambda_{j_1} \sim \lambda_{j_2}\right\}}$.

For every $m \leq 1$, the fixed particle number measure $M^{t,\epsilon,m,h}$ is finite due to the boundness of h, while since $\varepsilon > 0$, the measure $M^{t,\epsilon,m,h}$ is null for m sufficiently large, due to initial exclusion. We have shown therefore that $M^{t,\epsilon,h}$ is a finite measure. The condition of theorem is satisfied by choosing a suitable constant a.

Let F be defined by

$$F(\lambda_1, \dots, \lambda_l) = \begin{cases} 1, & \text{if } l = 1, \\ \frac{1}{l!} \sum_{G \in \mathcal{C}_l} \prod_{(j_1, j_2) \in G} \left(-\mathbf{1}_{\left\{\lambda_{j_1} \sim \lambda_{j_2}\right\}}\right), & \text{otherwise.} \end{cases} \tag{8}$$

Remark. We form the graph with vertices $\lambda_1, \dots, \lambda_l$, and let λ_{j_1} be connected to λ_{j_2} by an edge if and only if $\lambda_{j_1} \sim \lambda_{j_2}$. It is noteworthy that F is non-zero only if the graph formed is a connected graph. This imposes strong constraints on the packet configurations and compensates the factor μ_ε^{l-1} in the Boltzmann-Grad limit, as we will prove in the next section.

The following bound will be useful

Proposition 1 (Tree inequality, [2])**.**

$$\left|F\left(\lambda_1, \dots, \lambda_l\right)\right| \leq \frac{1}{l!} \sum_{T \in \mathcal{T}_n} \prod_{\{j_1, j_2\} \in E(T)} \mathbf{1}_{\lambda_{j_1} \sim \lambda_{j_2}}. \tag{9}$$

We have the following cluster expansion of the biased partition function of hard-sphere dynamics,

$$\mu_\varepsilon^{-1} \log \mathcal{Z}^{t,\varepsilon,h} = \sum_{l=1}^{\infty} \mu_\varepsilon^{l-1} \tag{10}$$

$$\prod_{k=1}^{l} \left(\int dv_{\lambda_j} \int dx^1_{\lambda_j} \int dM^{t,\varepsilon,|\lambda_j|} \exp \sum_{i\in\lambda_j} h\left(\mathbf{z}_i^\varepsilon\left(t\right)\right) \prod_{i\in\lambda_j} f^0\left(z_i\right) \right) F\left(\lambda_1, \dots, \lambda_l\right).$$

We intentionally moved a factor μ_ε to the left hand side in order to obtain a non-trivial limit (neither 0 nor infinity) under Boltzmann-Grad.

4. Diagrammatics

In this section, we will represent the "giant" integration

$$\int \prod_{k=1}^{l} \left(dv_{\lambda_j} dx^1_{\lambda_j} dM^{t,\varepsilon,|\lambda_j|} \exp \sum_{i\in\lambda_j} h\left(\mathbf{z}^\varepsilon_i(t)\right) \prod_{i\in\lambda_j} f^0\left(z_i\right) \right) F\left(\lambda_1,\ldots,\lambda_l\right)$$

in diagrams, by analyzing how the conditions $X_\lambda, F\left(\lambda_1,\ldots,\lambda_n\right)$ are realized. In fact, despite these being strong constraints, we can find an alternative set of parameters to recover some independence between the positions of particles.

Suppose throughout the subsection that we fix a time interval $[0,t]$ and have l packets $\lambda_1,\ldots,\lambda_l$ of size $m_1,\ldots,m_l$ respectively. We will change only the parameters on the position part, which is to say, throughout the subsection, we will condition on the fixed set of initial velocities $v_{\lambda_1},\ldots,v_{\lambda_l}$ (to recall, v_{λ_1} is the ordered list of initial velocities of particles in λ_1, for exmaple).

4.1. **Change of internal parameters of a packet.** From now on we consider only the packet λ_1. Without loss of generality suppose $\lambda_1 = \{1,\ldots,m_1\}$. By translational invariance, the packet dynamics relative to a fixed particle in the packet is independent of the initial position of the packet. Pick the particle in the packet with the smallest index, whose its initial position is $x^1_{\lambda_1}$. We condition on this variable. The rest of integration is perform on relative initial position variables

$$x^{\mathrm{int}}_\lambda = \left(x^2_{\lambda_1} - x^1_{\lambda_1},\ldots,x^m_{\lambda_1} - x^1_{\lambda_1}\right).$$

To better encode the constraints $\mathrm{IE}_{\lambda_1} X_{\lambda_1}$ (IE for initial exclusion and X for packet connectedness), we define the following for a packet λ_1.

Definition 8. For an initial configuration z_{λ_1} of packet λ_1 satisfying the initial exlusion constraint IE_{λ_1} (so that the dynamics is well-defined), we define the clustering collisions of the packet iteratively as follows.

(1) The *first clustering collision* is the first collision between particles in λ_1. We denoted by $\{i_1,i'_1\}$ the set of the first two particles. The time of this collision is denoted by $t_{\mathrm{col},1}$.
(2) For $k \le 2$, the *k-th clustering collision* is the first collision after the $k-1$-th clustering collision (that is to say after $t_{\mathrm{col},k-1}$) such that

$$\{i_1,i'_1\},\ldots,\left\{i_{k-1},i'_{k-1}\right\},\{i_k,i'_k\}$$

do not form a loop. In other words, collisions between particles who are already connected through a chain of collisions do not count. The time of this collision is denoted by $t_{\mathrm{col},k}$.

Conventionally for *k-th clustering edge* $\{i_k,i'_k\}$, we set $i_k > i'_k$. This allows us to write ordered list (i_k,i'_k) instead of unordered.

To each z_{λ_1} we associate a graph with ordered edges $T^\prec_{\lambda_1}$, whose vertex set is λ_1 and whose edges are ordered as follows

$$\{i_1,i'_1\} \prec \{i_2,i'_2\} \prec \cdots \prec \{i_c,i'_c\},$$

where c is the number of clustering collision before time t. By the definition of clustering recollision, this graph must be a tree. This is called *clustering collision tree.*

For k-th clustering collision, we define the *k-th clustering relative position* to be

$$\hat{x}_k = x_{i'_k} - x_{i_k}, \tag{11}$$

and the *k-th clustering impact parameter* to be

$$\omega_{\mathrm{col},k} = \frac{1}{\varepsilon}\left(x_{i'_k}\left(t_{\mathrm{col},k}\right) - x_{i_k}\left(t_{\mathrm{col},k}\right)\right). \tag{12}$$

We immediately have the following

Proposition 2. *If z_{λ_1} satisfies furthermore the connectedness condition X_{λ_1}, the number of clustering collisions is $m_1 - 1$, and $T^{\prec}_{\lambda_1}$ is a minimally connected tree on $\{1, \ldots, m_1\}$.*

Conversely, if the graph associated to z_{λ_1} is connected, z_{λ_1} is connected by collision.

We introduce the following notion which will be useful.

Definition 9 (Merged subclusters)**.** Suppose $m_1 \geq 1$ and $\lambda_1 = \{1, \ldots, m_1\}$. Merged subclusters of λ_1 are a sequence $\left\{\lambda_{(k)}, \lambda'_{(k)}\right\}_{1\leq k\leq m-1}$ obtained in the following iterative way:

(1) Start with discrete subclusters $L_0 = \{\{1\}, \ldots, \{m_1\}\}$.
(2) The first two subclusters $\lambda_{(1)}, \lambda'_{(1)}$ are distinct single element sets in L_0, i.e. for some $1 \leq i_1 \neq i'_1 \leq m$, we have $\lambda_{(1)} = \{i\}, \lambda'_{(1)} = \{i'\}$; merge these two elements into a single cluster $c_1 := \lambda_{(1)} \cup \lambda'_{(1)} = \{i_1, i'_1\}$; set $L_1 = \{c_1\} \cup \left(L_0 \setminus \left\{\lambda_{(1)}, \lambda'_{(1)}\right\}\right)$.
(3) At each step $k > 1$, choose two distinct elements $\lambda_{(k)}, \lambda'_{(k)}$ of L_{k-1}; merge them into $c_k = \lambda_{(1)} \cup \lambda'_{(1)}$; set $L_k = \{c_k\} \cup \left(L_{k-1} \setminus \left\{\lambda_{(k)}, \lambda'_{(k)}\right\}\right)$.

Conventionally we set $\max \lambda_{(k)} > \max \lambda'_{(k)}$ so that we can write ordered lists instead of unordered ones.

Let $\mathcal{T}^{\prec}_{m_1}$ be the set of connected tree with ordered edges on $\{1, \ldots m_1\}$.

Definition 10 (Merged subclusters corresponding to a collision tree)**.** To each tree $T \in \mathcal{T}^{\prec}_{m_1}$, we can associate a merged subcluster in the following iterative way:

In the step $k \geq 1$, merge the two clusters $\lambda_{(k)}, \lambda'_{(k)}$ in L_{k-1} which contain i_k, i'_k; form the new cluster; set the new set L_k.

Now we have a set of the discrete variable $T^{\prec}_{\lambda_1}$ and continuous variables $(x_k)_{k=1}^{m_1-1}$ which is equivalent to the old relative parameters $x^2_{\lambda_1} - x^1_{\lambda_1}, \ldots, x^{m_1}_{\lambda_1} - x^1_{\lambda_1}$.

Proposition 3. *Suppose $T \in \mathcal{T}^{\prec}_{m_1}$. Let $\left(\lambda_{(k)}, \lambda'_{(k)}\right)_{1\leq k\leq m-1}$ be the associated merged subclusters. For internal position variables*

$$x^{int}_{\lambda_1} = \left(x^2_{\lambda_1} - x^1_{\lambda_1}, \ldots, x^{m_1}_{\lambda_1} - x^1_{\lambda_1}\right)$$

satisfying conditions IE_{λ_1}, the map to clustering relative positions

$$\{\mathrm{IE}_{\lambda_1} = 1\} \cap \left\{T^{\prec}_{\lambda_1} = T\right\} \ni x^*_{\lambda_1} \mapsto (\hat{x}_1, \ldots, \hat{x}_{m_1-1}) \in \mathbb{R}^{m_1-1}$$

is linear and of Jacobian ± 1 (therefore is one-to-one). Furthermore, the image set can be descibed in the following iterative way:

(1) *The first clustering relative position $\hat{x}_1$ is such that particles i_1, i'_1 do not overlap at time zero, i.e. $|\hat{x}_1| > \varepsilon$.*
(2) *The k-th clustering relative position $\hat{x}_k$ is such that $\lambda_{(k)}, \lambda'_{(k)}$ collide and collide only after time $t_{col,k-1}$ and that i_k, i'_k are the first two particles in the two subclusters who collide.*

One can further express the relative initial position by the time and angle of collision.

Proposition 4. *Fixing the clustering collision tree. Let $t_{col,k}$ be the k-th clustering collision time and $v_{col,k}, v'_{col,k}$ be the velocities* before *collision of the two particles realizing the k-th clustering collision. We have that $v_{col,k}, v'_{col,k}$ is only dependent of $t_{col,1}, \omega_{col,1}, \ldots, t_{col,k-1}, \omega_{col,k-1}$, i.e. the collision velocity will only depend on information of the preceding collisions.*

Then $x^{int}_{\lambda_1}$ is in bijection with $t_{col,1}, \omega_{col,1}, \ldots, t_{col,m_1-1}, \omega_{col,m_1-1}$.

Moreover, the Jacobian of transformation is given by

$$dx^{int}_{\lambda_1} = \prod_{k=1}^{n-1} \left(\left(v_{col,k} - v'_{col,k} \right) \cdot \omega_{col,k} \right)_+ .$$

For notational convenience we denote

$$\mathcal{C}\left(v_1, v_2, \omega\right) = \left((v_1 - v_2) \cdot \omega \right)_+ .$$

4.2. **Change of absolute position parameters of packets.** In this subsection we will condition on the initial velocities v_{λ_j} and internal positions $x^{\mathrm{int}}_{\lambda_j}$ of the packets.

We first notice that

$$F\left(\lambda_1, \ldots, \lambda_l\right) = \frac{1}{l!} \sum_{G \in \mathcal{C}_l} \prod_{(j_1, j_2) \in G} \left(-\mathbf{1}_{\left\{\lambda_{j_1} \sim \lambda_{j_2}\right\}} \right)$$

is non-zero only if the overlapping relation forms a connected graph on the set $\{\lambda_1, \ldots, \lambda_l\}$. Thus the tree decomposition technique of the previous subsection can be applied, with only a minor modification. Since there may be more than one particles in a packet, a packet overlapping $\lambda \sim \lambda'$ can be realized by different pairs of particles $(i, i') \in (\lambda, \lambda')$. One need to sum these possibilities up when integrating. Considering this, we can obtain the following similar result.

Proposition 5. *One can define* clustering overlappings *by replacing all "collisions" by "overlappings", all "particles" by "packets" in Definition 8. The clustering overlapping times $t_{ov,k}$, angles $\omega_{ov,k}$ and tree $T^{\prec} \in \mathcal{T}^{\prec}_l$ can be analogously defined. We denote by $\lambda_{ov,k}, \lambda'_{ov,k}$ the two packets realizing the k-th clustering overlapping.*

Moreover, let $i_k \in \lambda_{ov,k}, i'_{ov,k}$ be the particles in respective packets realizing the overlapping, and $v_{ov,k}, v'_{ov,k}$ be the velocities of the particles when they overlap, we *have*

$$dx_{\lambda_1}^1 \cdots dx_{\lambda_l}^1 = \sum_{\substack{i_k\in\lambda_k, i'_k\in\lambda'_k \\ k=1,\ldots,l-1}} dx_{\lambda_1}^1 \prod_{k=1}^{l-1} dt_{ov,k} d\omega_{ov,k} \mathcal{C}\left(v_{ov,k}, v'_{ov,k}, \omega_{ov,k}\right)$$

$$= \sum_{\substack{i_k\in\lambda_k, i'_k\in\lambda'_k \\ k=1,\ldots,l-1}} dx_{\lambda_1}^1 \prod_{k=1}^{l-1} dt_{ov,k} d\omega_{ov,k} \left(\left(v_{ov,k} - v'_{ov,k}\right)\cdot \omega_{ov,k}\right).$$

4.3. **Representation of hard sphere dynamics in diagrams.** We sum up the results from the previous two subsection. To calculate $\mu_\varepsilon^{-1} \log \mathcal{Z}^{t,\varepsilon}(h)$, we need to

(1) Pick $l \geq 1$ and $m_1, \ldots, m_l \geq 1$. This corresponds to l clusters $\lambda_1, \ldots, \lambda_l$ of size $m_1, \ldots, m_l$ respectively.
(2) Pick initial velocities of particles in these clusters.
(3) Pick also a position $x_{\lambda_1}^1$.
(4) Pick an ordered tree $T_{\mathrm{ov}}^{\prec}$, and other l ordered tree $T_{\mathrm{col},k}^{\prec}, k = 1, \ldots, l$.
(5) For each edge of each tree, attach a collision or overlapping time and angle, and the times must respect the order of edges. *One must exclude all parameters which lead to collision or overlapping trees different from the assigned ones.*
(6) Add dynamical factors $\mathcal{C}\left(v_{\mathrm{col},k}, v'_{\mathrm{col},k}, \omega_{\mathrm{col},k}\right), \mathcal{C}\left(v_{\mathrm{ov},k}, v'_{\mathrm{ov},k}, \omega_{\mathrm{ov},k}\right)$ for all edges.
(7) Add factor combinatorial $F(\lambda_1, \ldots, \lambda_l)$ which *needs to be calculated from all overlappings, not just clustering overlappings.*
(8) Add combinatorial factor $\frac{1}{m_k!}, k = 1, \ldots, l$ for each collision tree.
(9) Calculate factors $\exp h, f^0$ according to the dynamics and add them.
(10) Finally, integrate all the variables.

Remark. Our integration scheme is still not satisfactory since we need to exclude all the "bad" parameters leading the different clustering trees. Besides, the combinatorial factor $F(\lambda_1, \ldots, \lambda_l)$ depends not only on the clustering overlapping tree $T_{\mathrm{ov}}^{\prec}$, since there may be non-clustering overlappings.

These problems will be eliminated when we take the limit $\varepsilon \to 0$, as more than $m_1 - 1$ collisions between m_1 particles, and more than $l - 1$ overlapping between l packets, are extremely rare events, whose probability goes to zero in the limit.

5. Limiting dynamics

In this section we give a representation of the hard-sphere dynamics in the Boltzmann-Grad limit $\varepsilon \to 0$. To be precise, we claim the following

Theorem 3. *There exists a positive time $T^\star$ (depending only on C_0, β_0) such that the limit*

$$\mathcal{J}(t,h) := \lim_{\varepsilon\to 0} \mu_\varepsilon^{-1} \log \mathcal{Z}^{t,\varepsilon,h}$$

exists for all $h : \mathbb{D} \to \mathbb{R}$ satisfying

$$|h| + |v \cdot \nabla_x h| \leq 1$$

and all time $t \in [0, T^\star)$.

Moreover, we can calculate $\mathcal{J}(t,h)$ by the following procedure.

(1) *Pick* $l \geq 1$ *and* $m_1, \ldots, m_l \geq 1$. *This corresponds to* l *clusters* $\lambda_1, \ldots, \lambda_l$ *of size* $m_1, \ldots, m_l$ *respectively.*
(2) *Pick initial velocities of particles in these clusters.*
(3) *Pick also a position* $x^1_{\lambda_1}$.
(4) *Pick an ordered tree* $T^{\prec}_{ov}$, *and other* l *ordered tree* $T^{\prec}_{col,k}, k = 1, \ldots, l$.
(5) *For each edge of each tree, attach a collision or overlapping time and angle, and the times must respect the order of edges.*
(6) *Add dynamical factors* $\mathcal{C}\left(v_{col,k}, v'_{col,k}, \omega_{col,k}\right), \mathcal{C}\left(v_{ov,k}, v'_{ov,k}, \omega_{ov,k}\right)$ *for all edges.*
(7) *Add combinatorial factor* $\frac{(-1)^{l-1}}{l!}$ *for the overlapping tree.*
(8) *Add combinatorial factor* $\frac{1}{m_k!}, k = 1, \ldots, l$ *for each collision tree.*
(9) *Calculate factors* $\exp h, f^0$ *according to the dynamics and add them.*
(10) *Finally, integrate all the variables.*

We will develop necessary technical tools in Section 6 and prove the theorem in Section 7.

6. Uniform L^1 bound and reduction to minimal trees

This is the most technical section of this mémoire. In the first part, we will prove an L^1 bound of each term in the cluster expansion of the hard sphere dynamics, which is uniform in ε. Guaranteed a uniform bound, we can to work term by term to prove the convergence claimed in Section 5. It will also be useful when we derive the macroscopic evolution of the system in Section 8. In the second part, we will argue that it is unlikely for m particles to have more than $m-1$ collisions, and for l packets to have more than $l-1$ overlappings, under the Boltzmann-Grad scaling. This probability will in fact go to zero when we take the limit $\varepsilon \to 0$, so will not contribute to the limiting dynamics.

6.1. **Uniform L^1 bound.**

In this subsection we employ the technique of *merged subforests* from [2] to prove the following uniform bounds on packet connectivity and overlappings.

We recall that the initial distribution function satisfies

$$\left|f^0(x,v)\right| + \left|\nabla_x f(x,v)\right| \leq C_0 \beta_0^{\frac{d}{2}} \exp\left(-\frac{\beta_0 v^2}{2}\right), \quad C_0 > 0, \beta_0 > 0.$$

Suppose in addition that the test function $h : \mathbb{D} \to \mathbb{R}$ is bounded: $|h| \leq C_1$.

Throughout the section we suppose that there are l packets of size $m_1, \ldots, m_l$ respectively. Let $m = m_1 + \cdots + m_l$, $\mathbb{V}^2 = \sum_{i \in \cup_{j=1}^l \lambda_j} v_i^2$ and $\mathbb{V}_S^2 = \sum_{i \in S} v_i^2$ for sets S containing particle indices.

First we will prove a simple inequality.

Lemma 4. *Let* I, J *be two finite index sets. Let* $(a_i)_{i \in I}, (b_j)_{j \in J}$ *be two real sequences. Moreover suppose* $(a'_i)_{i \in I}, \left(b'_j\right)_{j \in J}$ *are two sequences satisfying*

$$\sum_{i \in I} a_i^2 = \sum_{i \in I} \left(a'_i\right)^2, \quad \sum_{j \in J} b_j^2 = \sum_{j \in J} \left(b'_j\right)^2$$

Then for all $\beta > 0$ *We have the following inequality:*

$$\sum_{i \in I, j \in J} |a_i - b_j| \leq \frac{C}{\sqrt{\beta}} \sum_{i \in I, j \in J} \left(\beta \left(a'_i\right)^2 + 1\right)\left(\beta \left(b'_j\right)^2 + 1\right)$$

for some absolute constant $C > 0$.

Proof. Let $M = |I|, N = |J|$. Denote $A^2 = \sum_{i\in I} a_i^2, B^2 = \sum_{j\in J} b_i^2$.We have

$$\begin{aligned}
\text{LHS} &\le \sum_{i\in I}\sum_{j\in J} C\sqrt{a_i^2+b_j^2}\\
&\le C\sqrt{MN}\sqrt{\sum_{i\in I}\sum_{j\in J} a_i^2+b_j^2}\\
&= C\sqrt{MN}\sqrt{NA^2+MB^2}\\
&\le C\left(\sqrt{M}NA+\sqrt{N}MB\right)\\
&\le \frac{CMN}{\sqrt{\beta}}\left(\frac{\beta A^2}{M}+\frac{\beta B^2}{N}+1\right)\\
&\le \frac{C}{\sqrt{\beta}}\sum_{i\in I, j\in J}\left(\beta\left(a_i'\right)^2+1\right)\left(\beta\left(b_j'\right)^2+1\right) = \text{RHS}.
\end{aligned}$$

In the first and second inequalities we used Cauchy-Schwarz, in the third inequality we used $\sqrt{a+b} \le \sqrt{a}+\sqrt{b}$, and in the fourth inequality we used $x \le \frac{x^2+1}{2}$. $\square$

Proposition 6. *There exists an absolute constant C such that for all $\varepsilon > 0$, $x_{\lambda_1}^1 \in \mathbb{T}$, initial packet velocities $v_{\lambda_1}, \ldots, v_{\lambda_l}$ and all internal packet positions $x_{\lambda_1}^{int}, \ldots, x_{\lambda_1}^{int}$.*

$$\mu_\varepsilon^{l-1}\int dx_{\lambda_2}^1\cdots dx_{\lambda_l}^1\left|F\left(\lambda_1,\ldots,\lambda_l\right)\right|\left|\exp\sum_{i\in\cup_{j=1}^l\lambda_j} h\left(\mathbf{z}_i\left(t\right)\right)\right|\prod_{i\in\cup_{j=1}^l\lambda_j}\left|f^0\left(z_i\right)\right| \tag{13}$$

$$\le \left(C_0C_1\right)^m\left(\frac{Ct}{\sqrt{\beta_0}}\right)^{l-1}\frac{1}{l!}\sum_{T\in\mathcal{T}_l}\prod_{\left\{\lambda_{j_k},\lambda_{j_k'}\right\}\in E(T)}\sum_{i_k\in\lambda_{j_k}, i_k'\in\lambda_{j_k'}}\left(\beta_0 v_{i_k}^2+1\right)\left(\beta_0 v_{i_k'}^2+1\right)$$
$$\beta_0^{\frac{dm}{2}}\exp\left(-\frac{\beta_0}{2}\mathbb{V}^2\right).$$

Proof. According to the Proposition 1, the left hand side is bounded by

$$\text{LHS} \le \left(C_0C_1\right)^m\frac{\mu_\varepsilon^{l-1}}{l!}\int dx_{\lambda_2}^1\cdots dx_{\lambda_l}^1\sum_{T\in\mathcal{T}_n}\prod_{\{j_1,j_2\}\in E(T)}\mathbf{1}_{\lambda_{j_1}\sim\lambda_{j_2}}$$
$$\beta_0^{\frac{dm}{2}}\exp\left(-\frac{\beta_0}{2}\mathbb{V}^2\right).$$

Fixing T, we order the edges of T by the time when the corresponding overlapping takes place. That is to say, we define $\{j_1, j_2\} \prec \{j_1', j_2'\}$ if $\lambda_{j_1} \sim \lambda_{j_2}$ happens earlier than $\lambda_{j_1'} \sim \lambda_{j_2'}$. Then we let $t_{\mathrm{ov},1} < \cdots < t_{\mathrm{ov},l-1}$ be the corresponding time and let $\lambda_{\mathrm{ov},1}, \lambda_{\mathrm{ov},1}', \ldots, \lambda_{\mathrm{ov},l-1}, \lambda_{\mathrm{ov},l-1}'$ be the corresponding packets when these overlappings take place, with the convention that the index of $\lambda_{\mathrm{ov},k}$ is greater than $\lambda_{\mathrm{ov},k}'$. In this way the sum over T can be rewritten as

$$\sum_{T\in\mathcal{T}_l}\prod_{\{j_1,j_2\}\in E(T)}\mathbf{1}_{\lambda_{j_1}\sim\lambda_{j_2}} = \sum_{T^\prec\in\mathcal{T}_l^\prec}\mathbf{1}_{t_{\mathrm{ov},1}<\cdots<t_{\mathrm{ov},l-1}}\prod_{k=1}^{l-1}\mathbf{1}_{\lambda_{\mathrm{ov},k}\sim\lambda_{\mathrm{ov},k}'}.$$

Let $i_k \in \lambda_{\mathrm{ov},k}, i'_k \in \lambda'_{\mathrm{ov},k}$ be the two particles which realize the overlapping, and let $x_{\mathrm{ov},k}, x'_{\mathrm{ov},k}, v_{\mathrm{ov},k}, v'_{\mathrm{ov},k}$ be the velocities of the particles when the overlapping happens. Define

$$\omega_{\mathrm{ov},k} = \varepsilon^{-1}\left(x'_{\mathrm{ov},k} - x_{\mathrm{ov},k}\right).$$

The integration on absolute position of the packets can be transformed as follows

$$dx^1_{\lambda_1}\cdots dx^1_{\lambda_k} = dx^1_{\lambda_1}\prod_{k=1}^{l-1}\mu_\varepsilon^{-1} dt_{\mathrm{ov},k} d\omega_{\mathrm{ov},k}\left(\left(v_{\mathrm{ov},k} - v'_{\mathrm{ov},k}\right)\cdot\omega_{\mathrm{ov},k}\right)_+ .$$

The integration on the k-th overlapping variables $t_{\mathrm{ov},k}, \omega_{\mathrm{ov},k}$ is independent of all others, therefore we have

$$\begin{aligned}
&\frac{\mu_\varepsilon^{l-1}}{l!}\int dx^1_{\lambda_1}\cdots dx^1_{\lambda_l}\sum_{T\in\mathcal{T}_l}\prod_{\{j_1,j_2\}\in E(T)}\mathbf{1}_{\lambda_{j_1}\sim\lambda_{j_2}} \\
&\quad= \frac{\mu_\varepsilon^{l-1}}{l!}\int dx^1_{\lambda_1}\cdots dx^1_{\lambda_l}\sum_{T^\prec\in\mathcal{T}_l^\prec}\mathbf{1}_{t_{\mathrm{ov},1}<\cdots<t_{\mathrm{ov},l-1}}\prod_{k=1}^{l-1}\mathbf{1}_{\lambda_{\mathrm{ov},k}\sim\lambda'_{\mathrm{ov},k}} \\
&\quad= \frac{1}{l!}\int dx^1_{\lambda_1}\sum_{T^\prec\in\mathcal{T}_l^\prec} dt_{\mathrm{ov},1}\cdots dt_{\mathrm{ov},l-1}\mathbf{1}_{t_{\mathrm{ov},1}<\cdots<t_{\mathrm{ov},l-1}} \\
&\quad\cdot\prod_{k=1}^{l-1}\sum_{i_k\in\lambda_{\mathrm{ov},k},i'_k\in\lambda'_{\mathrm{ov},k}} d\omega_{\mathrm{ov},k}\left(\left(v_{i_k}\left(t_{\mathrm{ov},k}\right) - v_{i'_k}\left(t_{\mathrm{ov},k}\right)\right)\cdot\omega_{\mathrm{ov},k}\right)_+ \\
&\quad\le \frac{t^{l-1}}{l!}\sum_{T\in\mathcal{T}_l}\int\prod_{k=1}^{l-1}\sum_{i_k\in\lambda_{\mathrm{ov},k},i'_k\in\lambda'_{\mathrm{ov},k}} d\omega_{\mathrm{ov},k}\left(\left(v_{i_k}\left(t_{\mathrm{ov},k}\right) - v_{i'_k}\left(t_{\mathrm{ov},k}\right)\right)\cdot\omega_{\mathrm{ov},k}\right)_+ \\
&\quad\le \frac{(Ct)^{l-1}}{l!}\sum_{T\in\mathcal{T}_l}\int d\omega_{\mathrm{ov},1}\cdots d\omega_{\mathrm{ov},l-1} \\
&\qquad\cdot\prod_{k=1}^{l-1}\sum_{i_k\in\lambda_{\mathrm{ov},k},i'_k\in\lambda'_{\mathrm{ov},k}}\left|v_{i_k}\left(t_{\mathrm{ov},k}\right) - v_{i'_k}\left(t_{\mathrm{ov},k}\right)\right| \\
&\quad\le \frac{(Ct)^{l-1}}{l!}\sum_{T\in\mathcal{T}_l}\int d\omega_{\mathrm{ov},1}\cdots d\omega_{\mathrm{ov},l-1} \\
&\qquad\cdot\prod_{k=1}^{l-1}\frac{C}{\sqrt{\beta_0}}\sum_{i_k\in\lambda_{\mathrm{ov},k},i'_k\in\lambda'_{\mathrm{ov},k}}\left(\beta_0 v_{i_k}^2 + 1\right)\left(\beta_0 v_{i'_k}^2 + 1\right) \\
&\quad\le \left(\frac{Ct}{\sqrt{\beta_0}}\right)^{l-1}\frac{1}{l!}\sum_{T\in\mathcal{T}_l}\prod_{\left\{\lambda_{j_k},\lambda_{j'_k}\right\}\in E(T)}\sum_{i_k\in\lambda_{j_k},i'_k\in\lambda_{j'_k}}\left(\beta_0 v_{i_k}^2 + 1\right)\left(\beta_0 v_{i'_k}^2 + 1\right).
\end{aligned}$$

Note that in the last inequality we used the inequality in Proposition 4, with energy conservation

$$\sum_{i_k\in\lambda_{\mathrm{ov},k}}\left(v_{i_k}\left(t_{\mathrm{ov},k}\right)\right)^2 = \sum_{i_k\in\lambda_{\mathrm{ov},k}} v_{i_k}^2,$$

and similarly for $\lambda'_{\mathrm{ov},k}$. ∎

Proposition 7. *Let λ be a packet of size m. There exists an absolute constant $C>0$ such that for all x_λ^1, v_λ, we have that*

$$\begin{aligned}(14)\qquad &\frac{1}{m!}\sum_{T^{\prec}\in T_{m_1}^{\prec}}\int\prod_{k=1}^{m-1}dt_{col,k}d\omega_{col,k}\left|\mathcal{C}\left(v_{col,k},v'_{col,k},\omega_{col,k}\right)\right|\\ &\qquad\leq\frac{1}{m!}\left(\frac{Ct}{\sqrt{\beta_0}}\right)^{m-1}\sum_{T}\prod_{\{i,j\}\in E(T)}\left(\beta_0\left(v_i\right)^2+1\right)\left(\beta_0\left(v_j\right)^2+1\right).\end{aligned}$$

Proof. Let $\lambda_{(k)},\lambda'_{(k)}$ be the merged subclusters corresponding to $T^{\prec}$. We have that

$$\text{LHS}\leq\frac{1}{m!}\sum_{T^{\prec}\in T_{m_1}^{\prec}}\int\prod_{k=1}^{m-1}dt_{\text{col},k}d\omega_{\text{col},k}\left|v_{\text{col},k}-v'_{\text{col},k}\right|.\tag{15}$$

Note that the summation on trees can be replaced by summation on merged subclusters

$$\sum_{T^{\prec}\in T_{m_1}^{\prec}}\cdots=\sum_{\lambda_{(k)},\lambda'_{(k)}}\sum_{\substack{i_k\in\lambda_{(k)},i'_k\in\lambda'_{(k)}\\ k=1,\ldots,m-1}}\cdots.$$

For a choice of particles i_k,i'_k realizing the k-th (clustering) collision, we denote $v_{\text{col}}^{i_k},v_{\text{col}}^{i'_k}$ the velocities of the particles right before the collision. Thus we have

$$\begin{aligned}(16)\qquad &\sum_{T^{\prec}\in T_{m_1}^{\prec}}\int\prod_{k=1}^{m-1}dt_{\text{col},k}d\omega_{\text{col},k}\left|v_{\text{col},k}-v'_{\text{col},k}\right|\\ &\qquad=\sum_{\lambda_{(k)},\lambda'_{(k)}}\sum_{\substack{i_k\in\lambda_{(k)},i'_k\in\lambda'_{(k)}\\ k=1,\ldots,m-1}}\int\prod_{k=1}^{m-1}dt_{\text{col},k}d\omega_{\text{col},k}\left|v_{\text{col},k}-v'_{\text{col},k}\right|.\end{aligned}$$

Let $K_{\lambda_{(k)}},K_{\lambda'_{(k)}}$ be the size of subclusters $\lambda_{(k)},\lambda'_{(k)}$. We have according to Lemma 4,

$$\sum_{i_k\in\lambda_{(k)},i'_k\in\lambda'_{(k)}}\left|v_{\text{col},k}-v'_{\text{col},k}\right|\leq\frac{C}{\sqrt{\beta_0}}\sum_{i_k\in\lambda_{(k)},i'_k\in\lambda'_{(k)}}\left(\beta_0\left(v_{i_k}\right)^2+1\right)\left(\beta_0\left(v_{i'_k}\right)^2+1\right).$$

Note that

$$\begin{aligned}&\sum_{\lambda_{(k)},\lambda'_{(k)}}\prod_{k=1}^{m-1}\sum_{i_k\in\lambda_{(k)},i'_k\in\lambda'_{(k)}}\left(\left(\beta_0v_{i_k}\right)^2+1\right)\left(\beta_0\left(v_{i'_k}\right)^2+1\right)\\ (17)\qquad &=\sum_{T^{\prec}}\prod_{\{i,j\}\in E(T^{\prec})}\left(\beta_0\left(v_i\right)^2+1\right)\left(\beta_0\left(v_j\right)^2+1\right)\\ &=(m-1)!\sum_{T}\prod_{\{i,j\}\in E(T)}\left(\beta_0\left(v_i\right)^2+1\right)\left(\beta_0\left(v_j\right)^2+1\right).\end{aligned}$$

Combining equations (15, 16, 17), we have

$$
\begin{aligned}
\text{LHS} \leq & \frac{C^{m-1}(m-1)!}{m!} \sum_{T} \prod_{\{i,j\}\in E(T)} \\
& \cdot \int \prod_{k=1}^{m-1} dt_{\mathrm{col},k} d\omega_{\mathrm{col},k} \left(\beta_0 (v_i)^2+1\right)\left(\beta_0 (v_j)^2+1\right) \\
= & \frac{1}{m!}\left(\frac{Ct}{\sqrt{\beta_0}}\right)^{m-1} \sum_{T} \prod_{\{i,j\}\in E(T)} \left(\beta_0 (v_i)^2+1\right)\left(\beta_0 (v_j)^2+1\right) = \text{RHS}.
\end{aligned}
$$

□

Combining Propositions 6, 7, we have

Lemma 5. *There exists a $T^\star$ such that for all $t \in [0, T^\star)$, the sum and integration introduced in Definition 4.3 is absolutely convergent uniformly for all $\varepsilon > 0$.*

Proof. It remains to prove that

$$
\begin{aligned}
\sum_{l=1}^{\infty} \sum_{m_1,\ldots,m_l\geq 1} \int dV \exp\left(-\frac{\beta_0 \mathbb{V}^2}{2}\right) \frac{1}{l! m_1! \cdots m_l!} \left(C_0 C_1 \beta_0^{\frac{d}{2}}\right)^M \left(\frac{Ct}{\sqrt{\beta_0}}\right)^{M-1} \\
\sum_{T\in\mathcal{T}_l} \prod_{\left\{\lambda_{j_k},\lambda_{j'_k}\right\}\in E(T)} \sum_{i_k\in\lambda_{j_k}, i'_k\in\lambda_{j'_k}} \left(\beta_0 v_{i_k}^2+1\right)\left(\beta_0 v_{i'_k}^2+1\right) \\
\prod_{k=1}^{l} \sum_{T_k\in\mathcal{T}_{m_k}} \prod_{\{i,j\}\in E(T_k)} \left(\beta_0 v_i^2+1\right)\left(\beta_0 v_j^2+1\right)
\end{aligned}
$$

is convergent, where $\int dV$ means integration of all initial velocity variables.

Using the same technique as in Section 8.2 of [2], one can show that this is bounded by

$$
\sum_{l=1}^{\infty} \sum_{m_1,\ldots,m_l\geq 1} (C_0 C_1)^M \left(\frac{Ct}{\sqrt{\beta_0}}\right)^{M-1}
$$

upon a change of absolute constant C. Let $T^\star = \frac{1}{3}\frac{\sqrt{\beta_0}}{C_0 C_1 C}$, then for $t < T^\star$, the series is convergent. The desired result follows. □

6.2. **Reduction to minimal trees.** We claim without proof that the following propositions.

Proposition 8. *Let λ be a packet of size m. Then*

$$
\begin{aligned}
& \int dv_\lambda \exp\left(-\frac{\beta_0 \mathbb{V}_\lambda^2}{2}\right) \\
& \sum_{T^\prec\in\mathcal{T}_m^\prec} \prod_{k=1}^{m-1} dt_{col,k} d\omega_{col,k} \mathcal{C}\left(v_{col,k}, v'_{col,k}, \omega_{col,k}\right) \mathbf{1}_{more\ than\ m-1\ collisions} = O\left(\varepsilon^\alpha\right)
\end{aligned}
$$

for some $\alpha > 0$, where $\mathbb{V}_\lambda^2 = \sum_{i\in\lambda} v_i^2$ is the energy of the packet.

Proposition 9. *Let $\lambda_1, \ldots, \lambda_l$ be l packets, then*

$$\int dV \exp\left(-\frac{\beta_0 \mathbb{V}^2}{2}\right) \prod_{k=2}^{l} dx^1_{\lambda_k} \prod_{k=1}^{l} dM^{t,\varepsilon}\left(x^{int}_{\lambda_k}\right)$$
$$\sum_{T^{\prec} \in \mathcal{T}^{\prec}_m} \prod_{k=1}^{m-1} dt_{col,k} d\omega_{col,k} \mathcal{C}\left(v_{col,k}, v'_{col,k}, \omega_{col,k}\right) \mathbf{1}_{more\ than\ l-1\ overlappings}$$
$$= O\left(\varepsilon^{\delta}\right)$$

for some $\delta > 0$.

Thus we can remove the restriction and simplify Ursell function when we take the Boltzmann-Grad limit. To be precise, let $\mathcal{J}^{\varepsilon}(t,h)$ be the integration obtained by following procudures in Section 4.3, and let $\mathcal{K}^{\varepsilon}(t,h)$ be the integration obtained by integrating all domain and replacing $F(\lambda_1, \ldots, \lambda_l)$ by $\frac{(-1)^{l-1}}{l!}$. Then we have

Lemma 6.
$$\lim_{\varepsilon \to 0} \mathcal{K}^{\varepsilon}(t,h) - \mathcal{J}^{\varepsilon}(t,h) = 0.$$

7. Proof of convergence

Proof of Theorem 5. Let $\mathcal{J}(t,h)$ be the integration defined in Theorem 5. The existence (integrability) of $\mathcal{J}$ can be proved in exactly the same way that Lemma 5 is proved. According to Lemma 6, it suffices to show that

$$\lim_{\varepsilon \to 0} \mathcal{K}^{\varepsilon}(t,h) = \mathcal{J}(t,h).$$

Thanks to Lemma 5, we only need to show that when $\varepsilon \to 0$,

$$\prod_{i \in \cup_{j=1}^{l} \lambda_j} f^0\left(z^{\varepsilon}_i\right) \exp\left(\sum_{i \in \cup_{j=1}^{l} \lambda_j} h\left(\mathbf{z}^{\varepsilon}_i(t)\right)\right) \to \prod_{i \in \cup_{j=1}^{l} \lambda_j} f^0\left(z^0_i\right) \exp\left(\sum_{i \in \cup_{j=1}^{l} \lambda_j} h\left(\mathbf{z}^0_i(t)\right)\right), \tag{18}$$

and the rest will follow from dominated convergence theorem. Note that, since there are $m_1 + \cdots + m_l - 1$ overlappings and collisions in the dynamics, a particle's trajectory can at most deflect $m_1 + \cdots + m_l - 1$ times. Thus we have for all $t \in [0, T^{\star})$.

$$\left|\mathbf{x}^{\varepsilon}_i(t) - \mathbf{x}^0_i(t)\right| \leq (m_1 + \cdots + m_l - 1)\,\varepsilon,$$
$$\mathbf{v}^{\varepsilon}_i(t) = \mathbf{v}^0_i(t)$$

Using the regularity of f^0, h, we can derive the pointwise convergence (18). □

8. Macroscopic evolution equations

In this section we prove two macroscopic evolution equations of the hard sphere system. We will use the limiting dynamics introduction introduced in Section 5 to derive the Hamilton-Jacobi equation satisfied by the exponential moment. Then expanding Hamilton-Jacobi to first order, we can easily recover the Boltzmann equation. Our approach is different from Lanford's [5], who obtains directly the

Boltzmann equation by analyzing the evolution of distribution function. However, since Boltzmann is merely the first-order expansion of Hamilton-Jacobi, the latter contains much more information of the system's evolution than the former. Thus in this sense our approach is more general.

8.1. **Hamilton-Jacobi equation.**

Theorem 7. *According to Theorem 3, the following limit*

$$\lim_{\varepsilon\to 0}\mu_\varepsilon^{-1}\log\mathcal{Z}^{t,\varepsilon,h}$$

converges uniformly for all $t < C\sqrt{\beta_0} =: T^\star$ *and all function* h *satisfying the following bound*

$$|h(x,v)| + |\nabla_x h(x,v)| \le C_0 \exp\left(-\frac{\beta_0 v^2}{2}\right).$$

Denote $\gamma = \exp(h)$. *Define*

$$\mathcal{J}(t,\gamma) = \lim_{\varepsilon\to 0}\mu_\varepsilon^{-1}\log\mathcal{Z}^{t,\varepsilon,h} = \lim_{\varepsilon\to 0}\mu_\varepsilon^{-1}\log\mathcal{Z}^{t,\varepsilon,\log\gamma},$$

and let γ_t *be the solution of*

$$D_t\gamma_t = 0$$

with initial condition $\gamma_t|_{t=0} = \gamma$. *Then the limit* $\mathcal{J}$ *satisfies the following Hamilton-Jacobi equation for* $t \in [0, T^\star]$

$$\frac{\partial\mathcal{J}}{\partial t}(t,\gamma_t) = \\ \frac{1}{2}\int d\mu(z_1,z_2,\omega)\frac{\partial\mathcal{J}}{\partial\gamma}(t,\gamma_t)(z_1)\frac{\partial\mathcal{J}}{\partial\gamma}(t,\gamma_t)(z_2)\left(\gamma_t(z_1')\gamma_t(z_2') - \gamma_t(z_1)\gamma_t(z_2)\right),$$

where the notation is used

$$d\mu(z_1,z_2,\omega) := dv_1 dv_2 dx_1 dx_2 d\omega\delta_{x_1-x_2}\left((v_1-v_2)\cdot\omega\right)_+.$$

Proof. We express $\mathcal{J}$ using the packet representation

$$\mathcal{J}(t,\gamma_t) = \sum_{l=1}^{\infty}\frac{(-1)^{l-1}}{l!}\sum_{T_{\text{ov}}^{\prec}\in\mathcal{T}_l^{\prec}}\int dV dx_{\lambda_1}^1 dM^t(\lambda_1)\cdots dM^t(\lambda_k) \\ \cdot\sum_{\substack{i_k\in\lambda_{\text{ov},k}, i_k'\in\lambda_{\text{ov},k}\\ k=1,\dots,l-1}}\prod_{k=1}^{l-1}dt_{\text{ov},k}d\omega_{\text{ov},k}\left(\left(v_{\text{ov},k} - v_{\text{ov},k}'\right)\cdot\omega_{\text{ov},k}\right)_+ \\ \cdot\mathbf{1}_{0<t_{\text{ov},1}<\cdots<t_{\text{ov},l-1}<t}\exp\left(\sum_{k=1}^{l}\sum_{i\in\lambda_k}h_t(\mathbf{z}_i(t))\right),$$

where $\int dV$ means integration of all velocity variables in the initial condition. In three places the time variable t is involved. The first appears in the time-dependent test function h_t and the particle trajectory $\mathbf{z}_i(t)$. The second place is in the integration of overlapping time variables $t_{\text{ov},1},\dots,t_{\text{ov},l-1}$, where they are subject to the constraint

$$0 < t_{\text{ov},1} < \cdots < t_{\text{ov},l-1} < t.$$

The third place is in the packet measures dM^t, which can be written explicitly as

$$dM^t(\lambda_j) = \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{T^{\prec} \in \mathcal{T}_m^{\prec}} \prod_{k=1}^{m-1} dt_{j,\mathrm{col},k} d\omega_{j,\mathrm{col},k} \left((v_{j,\mathrm{col},k} - v_{j,\mathrm{col},k}) \cdot \omega_{j,\mathrm{col},k} \right)_+ \mathbf{1}_{0 < t_{j,\mathrm{col},1} < \cdots < t_{j,\mathrm{col},m-1} < t}.$$

Note that a similar constraint involving time t on collision times are also imposed.

Denote $\Delta\mathcal{J} := \mathcal{J}(t+\delta, h_{t+\delta}) - \mathcal{J}(t, h_t)$. We will show that it can be decomposed into three parts, plus a higher order term. Moreover, the three parts will correspond to the contribution from the three places identified above, respectively.

We let

$$\begin{aligned} \Delta_{\mathrm{transport}}\mathcal{J} := \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l!} \sum_{T_{\mathrm{ov}}^{\prec} \in \mathcal{T}_l^{\prec}} \int dV dx_{\lambda_1}^1 dM^t(\lambda_1) \cdots dM^t(\lambda_k) \\ \cdot \sum_{\substack{i_k \in \lambda_{\mathrm{ov},k}, i_k' \in \lambda_{\mathrm{ov},k} \\ k=1,\ldots,l-1}} \prod_{k=1}^{l-1} dt_{\mathrm{ov},k} d\omega_{\mathrm{ov},k} \left(\left(v_{\mathrm{ov},k} - v_{\mathrm{ov},k}' \right) \cdot \omega_{\mathrm{ov},k} \right)_+ \\ \cdot \exp\left(\sum_{k=1}^{l} \sum_{i \in \lambda_k} h_{t+\delta}(\mathbf{z}_i(t+\delta)) \right) - \mathcal{J}(t, h_t). \end{aligned}$$

That is to say, the difference between $\mathcal{J}$ with $h, \mathbf{z}$ changed but collision and overlapping times unchanged. Since during $s \in [t, t+\delta]$ the particles go straight with constant velocity, and h_t satisfies the free transport equation $D_t h_t = \partial_t h_t + v\partial_x h_t = 0$, we have that for all particles i, $h_{t+\delta}(\mathbf{z}_i(t+\delta)) = h_t(\mathbf{z}_i(t))$. Therefore $\Delta_{\mathrm{transport}}\mathcal{J} = 0$.

Similarly, we define

$$\begin{aligned} \Delta_{-}'\mathcal{J} := \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l!} \sum_{T_{\mathrm{ov}}^{\prec} \in \mathcal{T}_l^{\prec}} \int dV dx_{\lambda_1}^1 dM^t(z_{\lambda_1}) \cdots dM^t(z_{\lambda_k}) \\ \cdot \sum_{\substack{i_k \in \lambda_{\mathrm{ov},k}, i_k' \in \lambda_{\mathrm{ov},k} \\ k=1,\ldots,l-1}} \prod_{k=1}^{m-1} dt_{\mathrm{ov},k} d\omega_{\mathrm{ov},k} \left(\left(v_{\mathrm{ov},1} - v_{\mathrm{ov},k}' \right) \cdot \omega_{\mathrm{ov},k} \right)_+ \\ \cdot \exp\left(\sum_{k=1}^{l} \sum_{i \in \lambda_k} h_{t+\delta}(\mathbf{z}_i(t+\delta)) \right) \\ \cdot \left(\mathbf{1}_{\{0 < t_{\mathrm{ov},1} < \cdots < t_{\mathrm{ov},l-1} < t+\delta\}} - \mathbf{1}_{\{0 < t_{\mathrm{ov},1} < \cdots < t_{\mathrm{ov},l-1} < t\}} \right) \end{aligned}$$

and

$$\Delta'_{+}\mathcal{J} := \sum_{l=1}^{\infty}\frac{(-1)^{l-1}}{l!}\sum_{T_{\text{ov}}^{\prec}\in\mathcal{T}_l^{\prec}}\int dVdx_{\lambda_1}^1 dM^t(z_{\lambda_1})\cdots dM^t(z_{\lambda_k})$$

$$\cdot\sum_{\substack{i_k\in\lambda_{\text{ov},k},i'_k\in\lambda_{\text{ov},k}\\ k=1,\ldots,l-1}}\prod_{k=1}^{m-1}dt_{\text{ov},k}d\omega_{\text{ov},k}\left(\left(v_{\text{ov},1}-v'_{\text{ov},k}\right)\cdot\omega_{\text{ov},k}\right)_+$$

$$\cdot\exp\left(\sum_{k=1}^{l}\sum_{i\in\lambda_k}h_{t+\delta}\left(\mathbf{z}_i\left(t+\delta\right)\right)\right)$$

$$\cdot\left(\prod_{j=1}^{l}\mathbf{1}_{\{0<t_{j,\text{col},1}<\cdots<t_{j,\text{col},l-1}<t+\delta\}}-\prod_{j=1}^{l}\mathbf{1}_{\{0<t_{j,\text{col},1}<\cdots<t_{j,\text{col},l-1}<t\}}\right)$$

Using the uniform bounds Lemma 5 one can prove that indeed

$$\Delta\mathcal{J}=\Delta_{\text{transport}}\mathcal{J}+\Delta'_{-}\mathcal{J}+\Delta'_{+}\mathcal{J}+o\left(\delta\right)=\Delta'_{-}\mathcal{J}+\Delta'_{+}\mathcal{J}+o\left(\delta\right).$$

We now investigate the term $\Delta'_{-}\mathcal{J}$. Since the constraint on overlapping times is relaxed to

$$0<t_{\text{ov},1}<\cdots<t_{\text{ov},l-1}<t+\delta,$$

we are comparing the integration result on this new domain with the original. Denote $T_t=\{(t_1,\ldots,t_{l-1}):0<t_1<\ldots<t_{l-1}<t\}$. The difference is

$$T_{t+\delta}\backslash T_t=\{(t_1,\ldots,t_{l-1}):0<t_1\ldots<t_{l-2}<t<t_{l-1}<t+\delta\}\cup E,$$

where the measure of E is of $o\left(\delta\right)$. By using the L^1 bound, we can write that

$$\Delta'_{-}\mathcal{J}=\Delta_{-}\mathcal{J}+o\left(\delta\right)$$

where $\Delta_{-}\mathcal{J}$ is the integration on

$$\{(t_1,\ldots,t_{l-1}):0<t_1\ldots<t_{l-2}<t<t_{l-1}<t+\delta\}.$$

Thus,

$$\Delta_{-}\mathcal{J}=\sum_{l=1}^{\infty}\frac{(-1)^{l-1}}{l!}\int dVdM^t(z_{\lambda_1})\cdots dM^t(z_{\lambda_k})$$

$$\cdot\sum_{T_{\text{ov}}^{\prec}\in\mathcal{T}_l^{\prec}}\sum_{\substack{i_k\in\lambda_{\text{ov},k},i'_k\in\lambda_{\text{ov},k}\\ k=1,\ldots,l-1}}\prod_{k=1}^{l-1}dt_{\text{ov},k}d\omega_{\text{ov},k}\left(\left(v_{\text{ov},k}-v'_{\text{ov},k}\right)\cdot\omega_{\text{ov},k}\right)_+$$

$$\cdot\mathbf{1}_{0<t_{\text{ov},1}<\cdots<t_{\text{ov},l-2}<t}\mathbf{1}_{t<t_{\text{ov},l-1}<t+\delta}\exp\left(\sum_{k=1}^{l}\sum_{i\in\lambda_k}h_t\left(\mathbf{z}_i\left(t\right)\right)\right)$$

Notice that here we have replaced $h_{t+\delta}\left(\mathbf{z}_i\left(t+\delta\right)\right)$ by $h_t\left(\mathbf{z}_i\left(t\right)\right)$, since during no trajectory is deflected after an overlapping.

Conditioning on $l,V,\lambda_1,\ldots,\lambda_k$, we can delete the last edge of the overlapping tree $T_{\text{ov}}^{\prec}$, and split it into two trees, whose integrations are independent of each other. We call this operation *tree splitting*. To ease notation denote $\mathcal{C}\left(v,v',\omega\right)=\left(\left(v-v'\right)\cdot\omega\right)_+$.

Indeed,

$$\begin{aligned}
&\sum_{T_{\text{ov}}^{\prec}\in\mathcal{T}_l^{\prec}}\sum_{\substack{i_k\in\lambda_{\text{ov},k},i_k'\in\lambda_{\text{ov},k}\\k=1,\ldots,l-1}}\int\prod_{k=1}^{l-1}dt_{\text{ov},k}d\omega_{\text{ov},k}\mathcal{C}\left(v_{\text{ov},k},v_{\text{ov},k}',\omega_{\text{ov},k}\right)\\
&\quad\cdot\mathbf{1}_{0<t_{\text{ov},1}<\cdots<t_{\text{ov},l-2}<t}\mathbf{1}_{t<t_{\text{ov},l-1}<t+\delta}\exp H\\
=&\frac{1}{2}\sum_{\substack{\lambda,\lambda'\in\{\lambda_k\}_{k=1}^l\\\lambda\neq\lambda'}}\sum_{T_{\text{ov}}^{\prec}\in\mathcal{T}_l^{\prec}}\mathbf{1}_{\left\{\text{last edge of }T_{\text{ov}}^{\prec}\text{ is }\{\lambda,\lambda'\}\right\}}\sum_{\substack{i_k\in\lambda_{\text{ov},k},i_k'\in\lambda_{\text{ov},k}\\k=1,\ldots,l-1}}\\
&\quad\cdot\int\prod_{k=1}^{l-1}dt_{\text{ov},k}d\omega_{\text{ov},k}\mathcal{C}\left(v_{\text{ov},k},v_{\text{ov},k}',\omega_{\text{ov},k}\right)\\
&\quad\cdot\mathbf{1}_{0<t_{\text{ov},1}<\cdots<t_{\text{ov},l-2}<t}\mathbf{1}_{t<t_{\text{ov},l-1}<t+\delta}\exp H\\
=&\frac{1}{2}\sum_{\substack{\lambda,\lambda'\in\{\lambda_k\}_{k=1}^l\\\lambda\neq\lambda'}}\sum_{\substack{M\coprod N=\{\lambda_k\}_{k=1}^l\\\lambda\in M,\lambda'\in N}}\int\\
&\quad\cdot\sum_{T_M^{\prec}\in\mathcal{T}_M^{\prec}}\sum_{\substack{i_{M,k}\in\lambda_{\text{ov},M,k}\\i_{M,k}'\in\lambda_{\text{ov},M,k}'\\k\in M}}\prod_{k=1}^{|M|-1}dt_{\text{ov},M,k}d\omega_{\text{ov},M,k}\mathcal{C}\left(v_{\text{ov},M,k},v_{\text{ov},M,k}',\omega_{\text{ov},M,k}\right)\text{TO}_M\\
&\quad\cdot\sum_{T_N^{\prec}\in\mathcal{T}_N^{\prec}}\sum_{\substack{i_{N,k}\in\lambda_{\text{ov},N,k}\\i_{N,k}'\in\lambda_{\text{ov},N,k}'\\k\in N}}\prod_{k=1}^{|N|-1}dt_{\text{ov},N,k}d\omega_{\text{ov},N,k}\mathcal{C}\left(v_{\text{ov},N,k},v_{\text{ov},N,k}',\omega_{\text{ov},N,k}\right)\text{TO}_N\\
&\quad\cdot\sum_{\substack{i_{l-1}\in\lambda_{\text{ov},l-1}\\i_{l-1}'\in\lambda_{\text{ov},l-1}'}}dt_{\text{ov},l-1}d\omega_{\text{ov},l-1}\mathcal{C}\left(v_{\text{ov},l-1},v_{\text{ov},l-1}',\omega_{\text{ov},l-1}\right)\mathbf{1}_{t<t_{\text{ov},l-1}<t+\delta}\\
&\quad\cdot\exp H,
\end{aligned}$$

where $\exp H := \exp\left(\sum_{k=1}^l\sum_{i\in\lambda_k}h_t\left(\mathbf{z}_i\left(t\right)\right)\right)$, and $\text{TO}_{M,N}$ stands for the order condition of overlapping times in subclusters M,N, respectively. Here we used the independence of dynamics of M,N during time $s\in[0,t]$, more precisely, the fact that velocities $v_{\text{ov},M,k}$ depends only on overlapping parameters in M, i.e. $t_{\text{ov},M,l},\omega_{\text{ov},M,l},l=1,\ldots,k-1$, and the same to N. The double summation can also be exchanged

$$\begin{aligned}
\sum_{\substack{\lambda,\lambda'\in\{\lambda_k\}_{k=1}^l\\\lambda\neq\lambda'}}\sum_{\substack{M\dot\cup N=\{\lambda_k\}_{k=1}^l\\\lambda\in M,\lambda'\in N}}\cdots&=\sum_{M\dot\cup N=\{\lambda_k\}_{k=1}^l}\sum_{\lambda\in M,\lambda'\in N}\cdots\\
&=\sum_{l_1=1}^{l-1}\sum_{\substack{M\dot\cup N=\{\lambda_k\}_{k=1}^l\\|M|=l_1,|N|=l-l_1}}\sum_{\lambda\in M,\lambda'\in N}\cdots.
\end{aligned}$$

We now integrate with the conditionned variables $l, V, \lambda_1, \dots, \lambda_k$. Using symmetry with respect to permutations of $\lambda_1, \dots, \lambda_l$, we have

$$
\begin{aligned}
\Delta_- \mathcal{J} = \frac{1}{2} \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l!} \int dV dx^1_{\lambda_1} dM^t(\lambda_1) \cdots dM^t(\lambda_l) \sum_{l_1=1}^{l-1} \binom{l}{l_1} \\
\cdot \sum_{T^{\prec}_M \in \mathcal{T}^{\prec}_{l_1}} \sum_{\substack{i_{M,k} \in \lambda_{\mathrm{ov},M,k} \\ i'_{M,k} \in \lambda'_{\mathrm{ov},M,k} \\ k \in M}} \prod_{k=1}^{l_1-1} dt_{\mathrm{ov},M,k} d\omega_{\mathrm{ov},M,k} \mathcal{C}\left(v_{\mathrm{ov},M,k}, v'_{\mathrm{ov},M,k}, \omega_{\mathrm{ov},M,k}\right) \mathrm{TO}_M \\
\cdot \sum_{T^{\prec}_N \in \mathcal{T}^{\prec}_{l-l_1}} \sum_{\substack{i_{N,k} \in \lambda_{\mathrm{ov},N,k} \\ i'_{N,k} \in \lambda'_{\mathrm{ov},N,k} \\ k \in N}} \prod_{k=1}^{l-l_1-1} dt_{\mathrm{ov},N,k} d\omega_{\mathrm{ov},N,k} \mathcal{C}\left(v_{\mathrm{ov},N,k}, v'_{\mathrm{ov},N,k}, \omega_{\mathrm{ov},N,k}\right) \mathrm{TO}_N \\
\cdot \sum_{\substack{\lambda \in \{1,\dots,l_1\} \\ \lambda' \in \{l_1+1,\dots,l\}}} \sum_{i_{l-1} \in \lambda, i'_{l-1} \in \lambda'} dt_{\mathrm{ov},l-1} d\omega_{\mathrm{ov},l-1} \mathcal{C}\left(v_{\mathrm{ov},l-1}, v'_{\mathrm{ov},l-1}, \omega_{\mathrm{ov},l-1}\right) \\
\cdot \mathbf{1}_{t < t_{\mathrm{ov},l-1} < t+\delta} \exp H
\end{aligned}
$$

where we have fixed $M = \{1, \dots, l_1\}, N = \{l_1 + 1, \dots, l\}$. We can exchange summation

$$
\sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l!} \sum_{l_1=1}^{l-1} \binom{l}{l_1} \cdots = - \sum_{l_1=1}^{\infty} \frac{(-1)^{l_1-1}}{l_1!} \sum_{l_2=1}^{\infty} \frac{(-1)^{l_2-1}}{l_2!} \cdots
$$

with $l_2 = l - l_1$. This, in the end, gives us

$$
\begin{aligned}
\Delta_- \mathcal{J} = -\frac{1}{2} \sum_{l_1=1}^{\infty} \frac{(-1)^{l_1-1}}{l_1!} \sum_{l_2=1}^{\infty} \frac{(-1)^{l_2-1}}{l_2!} \int dV dx^1_{\lambda_1} \\
\cdot \prod_{k=1}^{l_1} dM^t(\lambda_k) \sum_{T^{\prec}_M \in \mathcal{T}^{\prec}_{l_1}} \sum_{\substack{i_{M,k} \in \lambda_{\mathrm{ov},M,k} \\ i'_{M,k} \in \lambda'_{\mathrm{ov},M,k} \\ k \in M}} \prod_{k=1}^{l_1-1} dt_{\mathrm{ov},M,k} d\omega_{\mathrm{ov},M,k} \mathcal{C}_M \, \mathrm{TO}_M \\
\cdot \prod_{k=1}^{l_2} dM^t(\mu_k) \sum_{T^{\prec}_N \in \mathcal{T}^{\prec}_{l_2}} \sum_{\substack{i_{N,k} \in \mu_{\mathrm{ov},N,k} \\ i'_{N,k} \in \mu'_{\mathrm{ov},N,k} \\ k \in N}} \prod_{k=1}^{l_2-1} dt_{\mathrm{ov},N,k} d\omega_{\mathrm{ov},N,k} \mathcal{C}_N \, \mathrm{TO}_N \\
\cdot \sum_{\substack{i \in \cup_{k=1}^{l_1} \lambda_k \\ i' \in \cup_{k=1}^{l_2} \mu_k}} d\omega_{\mathrm{ov}} \mathcal{C}\left(v_{\mathrm{ov}}, v'_{\mathrm{ov}}, \omega_{\mathrm{ov}}\right) \mathbf{1}_{t < t_{\mathrm{ov},l-1} < t+\delta} \exp H,
\end{aligned}
$$

where $\mathcal{C}_M := \prod_{k=1}^{l_1-1} \mathcal{C}\left(v_{\mathrm{ov},M,k}, v'_{\mathrm{ov},M,k}, \omega_{\mathrm{ov},M,k}\right)$ is the dynamical factor and similarly for N.

Note that in the Hamilton-Jacobi equation

$$\frac{\partial \mathcal{J}}{\partial \gamma}(t,\gamma)(z) = \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l!} \sum_{T_{\mathrm{ov}}^{\prec} \in \mathcal{T}_l^{\prec}} \int dV dx_{\lambda_1}^1 dM^t(\lambda_1) \cdots dM^t(\lambda_k)$$

$$\sum_{\substack{i_k \in \lambda_{\mathrm{ov},k}, i'_k \in \lambda_{\mathrm{ov},k} \\ k=1,\ldots,l-1}} \prod_{k=1}^{l-1} dt_{\mathrm{ov},k} d\omega_{\mathrm{ov},k} \mathcal{C}\left(v_{\mathrm{ov},k}, v'_{\mathrm{ov},k}, \omega_{\mathrm{ov},k}\right) \mathrm{TO}_{\{1,\ldots,k\}}$$

$$\sum_{i \in \cup_{k=1}^{l} \lambda_k} \delta_{\mathbf{z}_i(t)-z} \prod_{\substack{j \neq i \\ j \in \cup_{k=1}^{l} \lambda_k}} \gamma(\mathbf{z}_j(t)).$$

Therefore we have exactly the negative part of the right hand side.

The positive part can be recovered in an analogous way by splitting the trees in $\Delta_+\mathcal{J}$, the difference being that in case of collision, particles trajectories are deflected, and we no longer have$\mathbf{z}_i(t+) = \mathbf{z}_i(t)$. ☐

8.2. **Boltzmann equation.**

Definition 11. The distribution function F_1^ε of hard sphere dynamics is an almost everywhere defined function characterized by

$$\int_{\mathbb{D}} dz F_1^\varepsilon(t,z) h(z) := \frac{1}{\mu_\varepsilon} \mathbb{E}_\varepsilon \left[\sum_{i=1}^{\mathcal{N}} h(\mathbf{z}_i(t))\right]$$

for all smooth and compactly supported $h : \mathbb{D} \to \mathbb{R}$.

Proposition 10. *The distribution function of hard-sphere exists and is unique for all $\varepsilon > 0, t \geq 0$. Moreover, the function is bounded uniformly in ε, t.*

Proof. Uniqueness follows directly from the definition. For existence, one can condition on $\{\mathcal{N} = n\}$ and investigate the Liouville equation satisfied by the n particle distribution function $F^\varepsilon)_n$, from which follows of the existence and uniform boundedness of F_n^ε. The (one particle) distribution function is the marginal integration of the n particle one:

$$F_1^\varepsilon(z) = \int_{\mathbb{D}^{n-1}} dz_2 \cdots dz_n F_n^\varepsilon(z, z_2, \ldots, z_n).$$

More details can be found in [1]. ☐

The following formula relates exponential moment with distribution function.

Proposition 11. *For $h : \mathbb{D} \to \mathbb{R}$ smooth and compactedly supported, the function*

$$\Lambda_t^{\varepsilon,h}(\delta) = \frac{1}{\mu_\varepsilon} \log \mathbb{E}_\varepsilon \left[\exp\left(\delta \sum_{i=1}^{\mathcal{N}} h(\mathbf{z}_i(t))\right)\right]$$

is defined everywhere and analytic on $\mathbb{R}$. Moreover, we have

$$\frac{\partial \Lambda_t^{\varepsilon,h}}{\partial \delta}(0) = \frac{1}{\mu_\varepsilon} \mathbb{E}_\varepsilon \left[\sum_{i=1}^{\mathcal{N}} h(\mathbf{z}_i(t))\right] = \int_{\mathbb{D}} dz F_1^\varepsilon(t,z) h(z).$$

Proof. Expand the exponential by power series. The proposition follows directly by exchanging the expection and summation. ☐

Proposition 12. *For all smooth and compactedly supported $h : \mathbb{D} \to \mathbb{R}$ with $|h| + |\nabla_x h| \leq 1$, the limit*

$$\Lambda_t^h(\delta) = \lim_{\varepsilon \to 0} \Lambda_t^{\varepsilon,h}(\delta)$$

exists for $t < T^\star, \delta \in [-1,1]$ according to Theorem 3. We have also that it is analytic in δ on $[-1,1]$. Moreover, there exists a function F_1 such that we have

$$\int_{\mathbb{D}^n} dz F_1(t,z)\, h(z) = \frac{\partial \Lambda_t^h}{\partial \delta}(0),$$

and $F_1 = \lim_{\varepsilon \to 0} F_1^\varepsilon$.

Proof. The existence of limit is proved in Theorem 3, while the analyticity follows from the uniform L^1 bound. The bound also justifies that we can exchange the order of $\frac{\partial}{\partial \delta}$ and $\lim_{\varepsilon \to 0}$, therefore the limit

$$\lim_{\varepsilon \to 0} \int_{\mathbb{D}^n} dz F_1^\varepsilon(t,z)\, h(z) = \lim_{\varepsilon \to 0} \frac{\partial \Lambda_t^{\varepsilon,h}}{\partial \delta}(0) = \frac{\partial \Lambda_t^h}{\partial \delta}(0)$$

exists. Then a compactness argument, which is possible thanks to the uniform boundedness of F^ε, allows us to extract a subsequence and obtain F_1. □

We will consider F_1 as the distribution function of the limiting dynamics.

Theorem 8. *The function F_1 solves the following Boltzmann equation*

$$\frac{\partial f}{\partial t}(x,v,t) + v \cdot \nabla_x f(x,v,t) = \int dv_2 d\omega \left(f(x,v',t) f(x,v_2',t) - f(x,v,t) f(x,v_2,t) \right) \left((v - v_2) \cdot \omega \right)_+$$

in the distribution sense, with the initial condition $f|_{t=0} = f_0$.

Proof. Let $h : \mathbb{D} \to \mathbb{R}$ be a smooth and compactedly supported function satisfying

$$|h| + |\nabla_x h| \leq 1. \tag{19}$$

Define $\gamma_\delta = \exp(\delta h)$. Let h_t be the solution of $D_t h_t = 0$ with $h_t|_{t=0} = h$, $\gamma_{\delta,t} = \exp(\delta h_t)$ solves $D_t \gamma_{\delta,t} = 0$ and $\gamma_{\delta,0} = \gamma_\delta$. Then, according to Theorem 7, we have

$$\frac{\partial \mathcal{J}}{\partial t}(t,\gamma_{\delta,t}) = \frac{1}{2} \int d\mu(z_1,z_2,\omega) \frac{\partial \mathcal{J}}{\partial \gamma}(t,\gamma_{\delta,t})(z_1) \frac{\partial \mathcal{J}}{\partial \gamma}(t,\gamma_{\delta,t})(z_2) \left(\gamma_{\delta,t}(z_1') \gamma_{\delta,t}(z_2') - \gamma_{\delta,t}(z_1) \gamma_{\delta,t}(z_2) \right),$$

Note that

$$\mathcal{J}(t,\gamma_{\delta,t}) = \Lambda_t^{h_t}(\delta)$$

and according to proposition 12, we have also

$$\frac{\partial \mathcal{J}}{\partial \gamma}(t,\gamma = 1)(z) = F_1(t,z).$$

Again using the uniform L^1 bound, we can justify that

$$\begin{aligned}\left.\frac{\partial}{\partial\delta}\right|_{\delta=0}\frac{\partial\mathcal{J}}{\partial t}\left(t,\gamma_{\delta,t}\right) &= \frac{d}{dt}\left.\frac{\partial}{\partial\delta}\right|_{\delta=0}\mathcal{J}\left(t,\gamma_{\delta,t}\right)\\ &= \frac{d}{dt}\int_{\mathbb{D}}dzF_1\left(t,z\right)h_t\left(z\right),\\ \frac{\partial\mathcal{J}}{\partial\gamma}\left(t,\gamma_{\delta,t}\right)\left(z\right) &= F_1(t,z)+o\left(\delta\right),\end{aligned}$$

while $\gamma_{\delta,t}=\exp\left(\delta h_t\right)=1+\delta h_t+o\left(\delta\right)$.

Expanding both side of the Hamilton-Jacobi equation to the first order of δ, one finds

$$\begin{aligned}&\int_{\mathbb{D}}dz\frac{\partial F_1}{\partial t}\left(t,z\right)h_t\left(t,z\right)-\int_{\mathbb{D}}dzF_1\left(t,z\right)v\cdot\nabla_x h_t\left(t,z\right)=\frac{d}{dt}\int_{\mathbb{D}}dzF_1\left(t,z\right)h_t\left(z\right)\\ &\quad=\frac{1}{2}\int d\mu\left(z_1,z_2,\omega\right)F_1\left(t,z_1\right)F_1\left(t,z_2\right)\left(h_t\left(z_1'\right)+h_t\left(z_2'\right)-h_t\left(z_1\right)-h_t\left(z_2\right)\right),\\ &\quad=\frac{1}{2}\int dxdv_1dv_2d\omega\mathcal{C}\left(v_1,v_2,\omega\right)F\left(t,x,v_1\right)F\left(t,x,v_2\right)\\ &\qquad\cdot\left(h_t\left(x,v_1'\right)+h_t\left(x,v_2'\right)-h_t\left(x,v_1\right)-h_t\left(x,v_2\right)\right),\end{aligned}$$

which is in form of the Boltzman equation in distribution sense. Since $g=\left(g_{-t}\right)_t$, h_t can be any smooth and compacted support function satisfying bound (19). Our theorem is proved. □

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