OBSERVABLES AND STRONG ONE-SIDED CHAOS IN THE BOLTZMANN-GRAD LIMIT

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ABSTRACT. Boltzmann’s equation provides a microscopic model for the evolution of dilute classical gases. A fundamental problem in mathematical physics is to rigorously derive Boltzmann’s equation starting from Newton’s laws. In the 1970s, Oscar Lanford provided such a derivation, for the hard sphere interaction, on a small time interval. One of the subtleties of Lanford’s original proof was that the strength of convergence proven at positive times was much weaker than that which had to be assumed at the initial time, which is at odds with the idea of propagation of chaos. Several authors have addressed this situation with various notions of strong one-sided chaos, which is the true property which is propagated by the dynamics. We provide a new approach to the problem based on duality and the evolution of observables; the observables encode the detailed interaction and allow us to define a new notion of strong one-sided chaos.

1. Introduction

Kinetic theory is concerned with the description of dilute gases at the microscopic level. The fundamental equation of collisional kinetic theory is Boltzmann’s equation, which is an evolutionary partial differential equation (PDE) stated in terms of the phase-space density $f(t,x,v) \geq 0$. Boltzmann’s equation describes the effects of free transport and binary collisions between particles. In the case of hard spheres, Boltzmann’s equation is written

$$ (\partial_t + v \cdot \nabla_x) f(t,x,v) = Q(f,f)(t,x,v) $$

where $Q$ is the collision operator

$$ Q(f,f) = Q^+(f,f) - Q^-(f,f) $$

$$ Q^+(f,f) = \int_{\mathbb{R}^d \times S^{d-1}} [\omega \cdot (v_2 - v)]_+ f(t,x,v^*) f(t,x,v_2^*) dv_2 d\omega $$

$$ Q^-(f,f) = \int_{\mathbb{R}^d \times S^{d-1}} [\omega \cdot (v_2 - v)]_+ f(t,x,v) f(t,x,v_2) dv_2 d\omega $$

and

$$ v^* = v + \omega \cdot (v_2 - v) $$

$$ v_2^* = v_2 - \omega \cdot (v_2 - v) $$

We refer to [4] for a mathematical introduction to Boltzmann’s equation.

One of the central problems in kinetic theory is to derive Boltzmann’s equation starting from a system of $N$ particles interacting via a classical
Hamiltonian. For the hard sphere Boltzmann equation, the interaction is given by the hard sphere potential (billiard balls). The scaling limit in which one derives Boltzmann’s equation is known as the Boltzmann-Grad limit; in this limit, we have $N$ identical hard spheres of diameter $\varepsilon$, with $N \varepsilon^{d-1} = \ell^{-1}$ for some fixed $\ell > 0$. However, the Boltzmann-Grad scaling by itself does not force a Boltzmann type dynamics; it is also necessary to assume that the configurations of distinct particles are independent from one another at some initial time. Unfortunately, the independence between particles is not propagated by the $N$ particle dynamics. If independence breaks down at some positive time then the validation of Boltzmann’s equation is expected to fail. For this reason, one of the key problems in validating Boltzmann’s equation is to specify an appropriate notion of independence, or factorization, among particles.\footnote{More generally, it is possible to work with a notion of exchangeability in place of independence. In this case one derives statistical solutions of Boltzmann’s equation.}

Lanford has shown, in the 1970s, that if the particles are asymptotically decorrelated in a very strong sense at the initial time, then a weaker notion of factorization is propagated to positive times.\footnote{This is because the typical length scale for a collision is of order $\varepsilon$.} Indeed, Lanford assumes that the marginal associated to $s$ particles (for $s$ fixed) converges in $L^\infty$ at the initial time. This type of convergence cannot be propagated to positive times, for the following reason. If the marginals converge in $L^\infty$ at some positive time, then all we need to do is reverse the particle velocities and evolve forwards to again deduce Boltzmann’s equation on the time interval $[t, t + \tau)$. This is because $L^\infty$ is invariant under reversal of the velocities of all the particles. But if we reverse the particle velocities and evolve forwards then we should actually obtain the backwards Boltzmann equation (this is Boltzmann’s equation with a minus sign in front of $Q(f, f)$), because this is the only possibility which is consistent with the evolution we have already deduced on $[0, t]$. (This is due to the reversibility of Newton’s laws.) We refer to \footnote{More generally, it is possible to work with a notion of exchangeability in place of independence. In this case one derives statistical solutions of Boltzmann’s equation.} for a detailed discussion of the issue of irreversibility.

More generally, any norm which is invariant under reversal of particle velocities cannot be the correct norm for proving propagation of chaos, by the same argument. The essential conflict is that Newton’s laws are time-reversible whereas Boltzmann’s equation is irreversible (as evidenced by the $H$-theorem). This problem leads to the notion of strong one-sided chaos (strong chaos), which means that the topology of convergence in Lanford’s theorem should be sensitive only to particle configurations coming into a collision. (Indeed, after a collision, it is impossible for the particles to be completely decorrelated.) This already indicates that strong chaos must be a very subtle notion, because it implies that the dynamics is determined by the values of functions evaluated along very small subsets of their domain of definition.\footnote{This is because the typical length scale for a collision is of order $\varepsilon$.} To make matters worse, if we condition on the event that a collision does happen, then the set of points coming into the collision is
locally of the same measure as the set of points going out of the collision. This means that we cannot rely on abstract measure-theoretic notions of regularity; we must account for the details of the collision process.

The delicacy of the Boltzmann-Grad limit is the very reason that Lanford required the $L^\infty$ convergence of the data in the first place. It seems difficult to provide convergence at all scales, as Lanford’s theorem requires, without some type of $L^\infty$ norm. Multiple authors have refined Lanford’s theorem into a strong chaos result by proving uniform convergence along suitable subsets of the reduced phase space. We refer to [2, 5, 10, 12] and Appendix A of [14] for a variety of results concerning uniform convergence and strong chaos. The goal of the present work is to provide a new notion of strong chaos which is much weaker than those which have previously appeared in the literature. Instead of defining chaos via convergence relative to a single norm, we introduce a sequence of seminorms which capture information at different scales. Perhaps the most natural way to understand this new notion of chaos is to view it as the $L^1$ norm restricted to certain singular sets which arise from the dynamics.

**Organization of the paper.** In Section 2, we define basic notation following [6]. In Section 3, we define the BBGKY and dual BBGKY hierarchies, and quote several well-posedness results. We prove a comparison principle for solutions of the dual BBGKY hierarchy in Section 4. In Section 5, we use the dual BBGKY hierarchy to define singular sets which are associated with the hard sphere dynamics. In Section 6, we develop a connection between solutions of the dual BBGKY hierarchy and the traditional notion of a pseudo-trajectory. Finally, in Section 7, we state and prove our main result on the propagation of chaos.

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2. Notation

We will consider $N$ identical hard spheres in the spatial domain $\mathbb{R}^d$, $d \geq 2$. The spheres all have diameter $\varepsilon > 0$, their centers are located at positions $x_1, \ldots, x_N \in \mathbb{R}^d$, and their velocities are given by $v_1, \ldots, v_N \in \mathbb{R}^d$. The full configuration is written $Z_N = (X_N, V_N) = (x_1, \ldots, x_N, v_1, \ldots, v_N) \in [\mathbb{R}^d]^N \times [\mathbb{R}^d]^N$. 

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3We thank Mario Pulvirenti for pointing this out to us.
\( \mathbb{R}^{dN} \times \mathbb{R}^{dN} \). The \( N \) particle phase space is specified by the condition of exclusion of hard spheres:

\[
\mathcal{D}_N = \left\{ Z_N = (X_N, V_N) \in \mathbb{R}^{dN} \times \mathbb{R}^{dN} \mid \forall 1 \leq i < j \leq N, \ |x_i - x_j| > \varepsilon \right\}
\]  

(6)

As long as particles remain within \( \mathcal{D}_N \), they continue along free trajectories:

\[
\dot{X}_N = V_N, \quad \dot{V}_N = 0.
\]

If particles collide (i.e. \( Z_N \in \partial \mathcal{D}_N \)) then the velocities of the particles are transformed by the law of specular reflection, then the free evolution continues. The collective flow of \( N \) hard spheres is written \( \psi^t_N : \mathcal{D}_N \rightarrow \mathcal{D}_N \); this is a well-defined measurable measure-preserving map. \[1, 6\]

We always enforce the Boltzmann-Grad scaling \( N\varepsilon^{d-1} = \ell^{-1} \) for a fixed parameter \( \ell > 0 \). We will also require the reduced phase space \( \mathcal{D}_s \) for \( 1 \leq s \leq N \), which is the phase space of \( s \) identical hard spheres of diameter \( \varepsilon \); the map \( \psi^t_s : \mathcal{D}_s \rightarrow \mathcal{D}_s \) defines the flow of \( s \) hard spheres. If \( Z_s \in \partial \mathcal{D}_s \) then we denote by \( Z^*_s \) the image of \( Z_s \) under the collisional change of variables. In particular, if \( x_j = x_i + \varepsilon \omega \) then \( Z^*_s = (x_1, v_1, \ldots, x_i, v^*_i, \ldots, x_j, v^*_j, \ldots, x_s, v_s) \) where

\[
v^*_i = v_i + \omega \omega \cdot (v_j - v_i)
\]

\[
v^*_j = v_j - \omega \omega \cdot (v_j - v_i)
\]

We shall consider an initial density \( f_N(0) \in L^1(\mathcal{D}_N) \), which is non-negative, symmetric under particle interchange, and normalized so that \( \int_{\mathcal{D}_N} f_N(0, Z_N) dZ_N = 1 \). The evolved state \( f_N(t), t \geq 0 \), is defined as the pushforward of \( f_N(0) \) through \( \psi^t_N \). Since the hard sphere flow is measure-preserving, this means that

\[
f_N(t, Z_N) = f_N(0, \psi^{-t}_N Z_N)
\]  

(7)

We extend \( f_N(t) \) by zero to be defined on all of \( \mathbb{R}^{dN} \times \mathbb{R}^{dN} \). Since \( f_N(0) \) is symmetric under particle interchange, \( f_N(t) \) must be symmetric as well. We define the marginals \( f_N^{(s)}(t) \) for \( 1 \leq s \leq N \) by the formula

\[
f_N^{(s)}(t, Z_s) = \int_{\mathbb{R}^{d(N-s)} \times \mathbb{R}^{d(N-s)}} f_N(t, Z_N) dz_{s+1} \ldots dz_N
\]  

(8)

The symmetry of \( f_N \) implies that it does not matter which particles we integrate out, and the marginals are likewise symmetric under particle interchange. We also define

\[
E_s(Z_s) = \frac{1}{2} \sum_{i=1}^{s} |v_i|^2
\]  

\[
I_s(Z_s) = \frac{1}{2} \sum_{i=1}^{s} |x_i|^2
\]  

(9) (10)
3. The BBGKY and Dual BBGKY Hierarchies

Let \( f_N(t) \) be a solution of Liouville’s equation (for the hard sphere interaction), with marginals \( f^{(s)}_N(t) \) for \( 1 \leq s \leq N \). Then it is possible to show that the marginals obey the following hierarchy of equations, known as the BBGKY hierarchy (Bogoliubov-Born-Green-Kirkwood-Yvon):

\[
(\partial_t + V_s \cdot \nabla X_s) f^{(s)}_N(t, Z_s) = (N - s) \varepsilon^{d-1} C_{s+1} f^{(s+1)}_N(t, Z_{s+1}) \tag{11}
\]

Here \( f^{(s)}_N(t, Z_s) = f^{(s)}_N(t, Z_s) \) and the operator \( C_{s+1} \) is defined as follows:

\[
C_{s+1} = \sum_{i=1}^{s} \left( C_{i,s+1}^+ - C_{i,s+1}^- \right) \tag{12}
\]

\[
C_{i,s+1}^- f^{(s+1)}_N = \int_{\mathbb{R}^{d+1}} dv_{s+1} d\omega \left[ \omega \cdot (v_{s+1} - v_i) \right]_+ \times f_N^{(s+1)}(t, x_1, v_1, \ldots, x_i, v_i, \ldots, x_s, v_s, x_i + \varepsilon \omega, v_{s+1}) \tag{13}
\]

\[
C_{i,s+1}^+ f^{(s+1)}_N = \int_{\mathbb{R}^{d+1}} dv_{s+1} d\omega \left[ \omega \cdot (v_{s+1} - v_i) \right]_+ \times f_N^{(s+1)}(t, x_1, v_1, \ldots, x_i, v_i^*, \ldots, x_s, v_s, x_i + \varepsilon \omega, v_{s+1}^*) \tag{14}
\]

We remark that it is possible to consider solutions of the BBGKY hierarchy which do not arise as a consistent sequence of marginals. Such solutions are not necessarily physically meaningful (e.g. in general the BBGKY hierarchy does not preserve non-negativity of solutions). However, we will need to consider general solutions of the BBGKY hierarchy in order to define the so-called dual BBGKY hierarchy. We always assume that the functions \( f^{(s)}_N \) are symmetric under particle interchange.

Let \( \Phi_N = \left\{ \varphi^{(s)}_N \right\}_{1 \leq s \leq N} \) be a sequence of real-valued functions such that \( \varphi^{(s)}_N \) is defined on \( \mathcal{D}_s \) and symmetric under particle interchange. Furthermore, let \( F_N = \left\{ f^{(s)}_N \right\}_{1 \leq s \leq N} \) be a sequence of densities, again symmetric under particle interchange. Following [7], we introduce the following duality bracket:

\[
\langle \Phi_N, F_N \rangle = \sum_{s=1}^{N} \frac{1}{s!} \int_{\mathcal{D}_s} \varphi^{(s)}_N(Z_s) f^{(s)}_N(Z_s) dZ_s \tag{15}
\]

The dual BBGKY hierarchy is the evolution equation satisfied by the sequence of functions \( \Phi_N(t) \) under the condition that, for any solution \( F_N(t) \) of the BBGKY hierarchy, the following holds

\[
\langle \Phi_N(t), F_N(0) \rangle = \langle \Phi_N(0), F_N(t) \rangle \tag{16}
\]
It is possible to show, by elementary computation, that the dual BBGKY hierarchy for hard spheres is given by the following sequence of equations:

\[
(\partial_t - V_s \cdot \nabla X_s) \varphi_N^{(s)}(t, Z_s) = 0 \quad (Z_s \in \mathcal{D}_s, \ s = 1, \ldots, N) \tag{17}
\]

\[
\frac{\varphi_N^{(s)}(t, Z_s)}{N - s + 1} + \varphi_N^{(s-1)}(t, (Z_s^*)^{(i)}) + \varphi_N^{(s-1)}(t, (Z_s^*)^{(j)}) = \frac{\varphi_N^{(s)}(t, Z_s)}{N - s + 1} + \varphi_N^{(s-1)}(t, Z_s^{(i)}) + \varphi_N^{(s-1)}(t, Z_s^{(j)})
\]  \tag{18}

\[
\left( Z_s \in \left( \Sigma_s(i, j) \times \mathbb{R}^d s \right) \cap \partial \mathcal{D}_s, \ s = 2, \ldots, N \right)
\]

Here \(Z_s^{(i)} = (z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_s)\). The dual BBGKY hierarchy may be solved by applying induction on \(s\) and the method of characteristics. The value of \(\varphi_N^{(s)}\) is transported freely along characteristics between collisions. Across any collision, the value of \(\varphi_N^{(s)}\) experiences a “jump” which is determined by \(\varphi_N^{(s-1)}\). Since the evolution of \(\varphi_N^{(1)}\) is trivially determined, it is likewise possible to determine every \(\varphi_N^{(s)}\) inductively using Duhamel’s formula. We will sometimes refer to solutions of the dual BBGKY hierarchy as observables.

We will quote two local well posedness theorems for the dual BBGKY hierarchy. Both theorems are proven in \cite{Ryan1, Ryan2}, though the proofs are based heavily on classical proofs of well-posedness for the BBGKY hierarchy. \cite{Ryan1, Ryan2, Ryan3, Ryan4} We refer the reader to \cite{Ryan1, Ryan2, Ryan3, Ryan4, Ryan5} for standard well-posedness results concerning the BBGKY hierarchy. Given parameters \(\beta > 0, \mu \in \mathbb{R}\), let us define the norm

\[
\| \Phi_N \|_{\mathcal{L}^1_{\beta, \mu}} = \sum_{s=1}^{N} \frac{1}{s!} \int_{D_s} \left| \varphi_N^{(s)}(Z_s) \right| e^{-\beta E_s(Z_s)} e^{-\mu s} dZ_s \tag{19}
\]

**Theorem 3.1.** Suppose \(\Phi_N(0) = \left\{ \varphi_N^{(s)}(0, Z_s) \right\}_{1 \leq s \leq N}\) is a sequence of functions, with each \(\varphi_N^{(s)}(0)\) defined on \(\mathcal{D}_s\) and symmetric under particle interchange. Furthermore, suppose that \(\| \Phi_N(0) \|_{\mathcal{L}^1_{\beta, (\mu-1)}} < \infty\) for some \(\beta > 0, \mu \in \mathbb{R}\). There exists a constant \(C_d > 0\), depending only on \(d\), such that if \(T_L < C_d \ell e^{\mu \beta^{d+1}}\), then there exists a unique solution \(\Phi_N(t)\) of the dual BBGKY hierarchy for \(t \in [0, T_L]\) satisfying the bound

\[
\sup_{0 \leq t \leq T_L} \| \Phi_N(t) \|_{\mathcal{L}^1_{\beta, \mu}} \leq \| \Phi_N(0) \|_{\mathcal{L}^1_{\beta, (\mu-1)}} \tag{20}
\]

**Theorem 3.2.** If \(\ell^{-1} e^{-\mu \beta^{-\frac{d+1}{2}}}\) is sufficiently small (depending only on \(d\)) then for any \(T > 0\) we have the following: Suppose \(\Phi_N(0) = \left\{ \varphi_N^{(s)}(0, Z_s) \right\}_{1 \leq s \leq N}\) is a sequence of functions, with each \(\varphi_N^{(s)}(0)\) defined on \(\mathcal{D}_s\) and symmetric
under particle interchange. Further suppose that, for some \( \beta > 0 \) and \( \mu \in \mathbb{R} \), there holds

\[
\sum_{s=1}^{N} \frac{1}{s!} \int_{D_s} \left| \varphi_N^{(s)}(0, Z_s) \right| e^{-\beta (E_s(Z_s) + I_s(Z_s))} e^{-(\mu - 1)s} dZ_s < \infty
\]  

(21)

Then the dual BBGKY hierarchy has a unique solution for \( t \in [0, T] \) and it satisfies

\[
\sum_{s=1}^{N} \frac{1}{s!} \int_{D_s} \left| \varphi_N^{(s)}(T, Z_s) \right| e^{-\beta (E_s(Z_s) + I_s(Z_s))} e^{-\mu s} dZ_s 
\]

\[
\leq \sum_{s=1}^{N} \frac{1}{s!} \int_{D_s} \left| \varphi_N^{(s)}(0, Z_s) \right| e^{-\frac{1}{2}\beta (E_s(Z_s) + I_s(Z_s))} e^{-(\mu - 1)s} dZ_s
\]  

(22)

**Remark.** In the context of the original paper by Illner & Pulvirenti [8,9], the smallness condition in Theorem 3.2 is viewed as a largeness condition on the mean free path \( \ell \) (relative to \( f_0 \)), which in turn regulates the magnitude of the nonlinearity. In this sense, Theorem 3.2 is a “global-in-time” result which is valid for “small” initial data (i.e. small \( f_0 \)). However, it is also possible to view \( \ell \) as fixed, choose an arbitrary (compactly supported) initial observable \( \Phi_N(0) \), and then choose values of \( \beta, \mu \) which meet the smallness condition; this is always possible because \( \mu \) ranges over all of \( \mathbb{R} \). This gives us a way to make global sense of the dual BBGKY hierarchy for arbitrary observables.

It is important to realize that this does not allow us to relax the small time condition in Lanford’s theorem (for large \( f_0 \)) because not all observables can be paired against a given \( f_0 \) to yield a finite duality pairing. In order to make effective use of the global boundedness of observables, it is absolutely necessary to understand cancellation effects; such an understanding is well out of reach at the present time.

4. A Comparison Principle

The dual BBGKY hierarchy does not preserve positivity of solutions. It is easy to see that typical non-negative data \( \{ \varphi_N^{(s)}(0) \} \) will lead to solutions \( \{ \varphi_N^{(s)}(t) \} \) that cease to be non-negative for \( t > 0 \). Moreover, typical initial conditions lead to solutions that strongly concentrate on very small subsets of the phase space. On the other hand, very special initial conditions lead to trivial evolutions; for instance, we can let \( \varphi_N^{(s)}(0) = 1_{D_s} \) identically for all \( s \), then \( \varphi_N^{(s)}(t) = 1_{D_s} \) for all \( t > 0 \) and all \( s \). The goal of the present section is to construct an alternative hierarchy which controls the dual BBGKY hierarchy pointwise but which has better monotonicity properties.
The first step is to construct a lower envelope \( \underline{\varphi}_N^{(s)} \) and an upper envelope \( \overline{\varphi}_N^{(s)} \), which will control the dual BBGKY hierarchy from below and above. The lower and upper envelopes are, in turn, coupled to each other. The upper envelope solves the following evolution equation:

\[
(\partial_t - V_s \cdot \nabla_{X_s}) \overline{\varphi}_N^{(s)}(t, Z_s) = 0 \quad (Z_s \in D_s, s = 1, \ldots, N)
\]

\[
\frac{\overline{\varphi}_N^{(s)}(t, Z_s^*)}{N - s + 1} + \overline{\varphi}_N^{(s-1)}(t, (Z_s^*)^{(i)}) + \underline{\varphi}_N^{(s-1)}(t, (Z_s^*)^{(j)}) =
\]

\[
= \frac{\overline{\varphi}_N^{(s)}(t, Z_s)}{N - s + 1} + \overline{\varphi}_N^{(s-1)}(t, Z_s^{(i)}) + \overline{\varphi}_N^{(s-1)}(t, Z_s^{(j)})
\]

\[
\left( Z_s \in \left( N_s(i, j) \times \mathbb{R}^{ds} \right) \cap \partial D_s^{\text{post}}, \ s = 2, \ldots, N \right)
\]

The lower envelope, in turn, solves the following equation:

\[
(\partial_t - V_s \cdot \nabla_{X_s}) \underline{\varphi}_N^{(s)}(t, Z_s) = 0 \quad (Z_s \in D_s, s = 1, \ldots, N)
\]

\[
\frac{\underline{\varphi}_N^{(s)}(t, Z_s^*)}{N - s + 1} + \underline{\varphi}_N^{(s-1)}(t, (Z_s^*)^{(i)}) + \overline{\varphi}_N^{(s-1)}(t, (Z_s^*)^{(j)}) =
\]

\[
= \frac{\underline{\varphi}_N^{(s)}(t, Z_s)}{N - s + 1} + \underline{\varphi}_N^{(s-1)}(t, Z_s^{(i)}) + \underline{\varphi}_N^{(s-1)}(t, Z_s^{(j)})
\]

\[
\left( Z_s \in \left( N_s(i, j) \times \mathbb{R}^{ds} \right) \cap \partial D_s^{\text{post}}, \ s = 2, \ldots, N \right)
\]

We are able to prove the following result by elementary manipulations:

**Lemma 4.1.** Let \( 1 \leq S \leq N \) and assume that, for \( 1 \leq s \leq S \),

\[
\underline{\varphi}_N^{(s)}(0) \leq \varphi^{(s)}_N(0) \leq \overline{\varphi}_N^{(s)}(0)
\]

Then for all \( t \geq 0 \) and all \( 1 \leq s \leq S \),

\[
\underline{\varphi}_N^{(s)}(t) \leq \varphi^{(s)}_N(t) \leq \overline{\varphi}_N^{(s)}(t)
\]

**Proof.** Apply induction on \( S \). \( \square \)

**Remark.** Note that Lemma 4.1 is a very general result because the lower and upper envelopes still see cancellations and may not be non-negative.

Let us now define a new hierarchy which solves the following equation:

\[
(\partial_t - V_s \cdot \nabla_{X_s}) \varphi^{(s)}_N(t, Z_s) = 0 \quad (Z_s \in D_s, s = 1, \ldots, N)
\]

\[
\frac{\varphi^{(s)}_N(t, Z_s^*)}{N - s + 1} = \varphi^{(s-1)}_N(t, (Z_s^*)^{(i)}) - \varphi^{(s-1)}_N(t, (Z_s^*)^{(j)}) =
\]

\[
= \frac{\varphi^{(s)}_N(t, Z_s)}{N - s + 1} + \varphi^{(s-1)}_N(t, Z_s^{(i)}) + \varphi^{(s-1)}_N(t, Z_s^{(j)})
\]

\[
\left( Z_s \in \left( N_s(i, j) \times \mathbb{R}^{ds} \right) \cap \partial D_s^{\text{post}}, \ s = 2, \ldots, N \right)
\]
We assume $\hat{\varphi}^{(s)}(0) \geq 0$ for all $s$; then, the same holds for all $t > 0$. Then if $\varphi^{(s)}_N(t) = \hat{\varphi}^{(s)}_N(t)$ and $\hat{\varphi}^{(s)}_N(t) = -\varphi^{(s)}_N(t)$ for all $s$ then the functions $\varphi^{(s)}_N(t)$ and $\hat{\varphi}^{(s)}_N(t)$ solve the equations for upper and lower envelopes, respectively. In particular we deduce the following result:

**Lemma 4.2.** Let $1 \leq S \leq N$ and assume that, for $1 \leq s \leq S$,

$$ \left| \varphi^{(s)}_N(0) \right| \leq \hat{\varphi}^{(s)}_N(0) \quad (31) $$

Then for all $t \geq 0$ and all $1 \leq s \leq S$,

$$ \left| \varphi^{(s)}_N(t) \right| \leq \hat{\varphi}^{(s)}_N(t) \quad (32) $$

5. A Hierarchy of Singular Sets

The dynamics of the BBGKY hierarchy is determined by the initial data $f^{(s)}_N(0)$ evaluated along very singular subsets of the reduced phase space $D_s$. Our goal is to define these singular sets in an abstract fashion by relying on duality and Lemma 4.2. We will see that by choosing initial data $\hat{\varphi}^{(s)}_N(0)$ carefully, we can force the dual BBGKY hierarchy to identify the singular sets for us.

Let us define

$$ \hat{\varphi}^{(s)}_{N,j}(0) = \begin{cases} 1_{D_s} & \text{if } s = j \\ 0 & \text{otherwise} \end{cases} \quad (33) $$

We let $\varphi^{(s)}_{N,j}(t)$ solve $\partial_t \varphi^{(s)}_{N,j}(t) = \Delta \varphi^{(s)}_{N,j}(t)$. Note carefully that $\varphi^{(j+1)}_{N,j}(t)$ is, at each point, an integer multiple of $N - j$. Furthermore by 3, at any two points where $\varphi^{(j+1)}_{N,j}(t)$ is non-zero, it is separated by (at most) a constant multiple depending on $j$. To a good approximation, $\varphi^{(j+1)}_{N,j}(t)$ is a delta function concentrated on a subset (in fact a submanifold) of $D_{j+1}$. The easiest way to see this is that the dual BBGKY hierarchy (as well as the hierarchy satisfied by $\hat{\varphi}^{(s)}_N$) is well-posed in some weighted $L^1$ space. The Lebesgue measure of the support of $\varphi^{(s)}_{N,j}(t)$ is locally of order $O(N^{-1})$, which is $O(\varepsilon^{d-1})$ due to the Boltzmann-Grad scaling. This is consistent with the estimates provided in 2.

All the above considerations remain valid when applied to $\hat{\varphi}^{(s)}_{N,j}(t)$ for $s > j + 1$, except that we gain a power of $N$ pointwise each time we increment $s$ by one. The correct interpretation of this phenomenon is that we are isolating submanifolds of increasing codimension, due to an increasing number of collision constraints. In particular, the measure of the support of $\hat{\varphi}^{(s)}_{N,j}(t)$, for $s > j$, is locally of order $O(\varepsilon^{(s-j)(d-1)})$, which is again consistent with [2]. To summarize, for each $s \in \mathbb{N}$ and $N \gg s$, we have a hierarchy of singular sets given by the support of $\hat{\varphi}^{(s)}_{N,j}(t)$ for $t$ large and $1 \leq j < s$. These are exactly the sets which are relevant for the dynamics of the BBGKY hierarchy.
In the remainder of this section we will quantify the above considerations in a precise way. First we observe that the functions \( \hat{\varphi}^{(s)}_{N,j}(t) \) are increasing in time.

**Lemma 5.1.** For any \( 1 \leq j < s \), any \( 0 < t < t' \), and almost every \( Z_s \in \mathcal{D}_s \),

\[
\hat{\varphi}^{(s)}_{N,j}(t, Z_s) \leq \hat{\varphi}^{(s)}_{N,j}(t', Z_s) \tag{34}
\]

**Proof.** We write the Duhamel formula to express \( \hat{\varphi}^{(s)}_{N,j}(t, Z_s) \) in terms of \( \hat{\varphi}^{(s-1)}_{N,j} \); then apply induction on \( s \). The number of jumps in the Duhamel formula is non-decreasing in time, and the size of each jump is non-decreasing in time by the inductive hypothesis, hence the conclusion. \( \square \)

The functions \( \hat{\varphi}^{(s)}_{N,j}(t) \) range over a discrete set.

**Lemma 5.2.** For any \( 1 \leq s < j \) and any \( t > 0 \), \( \hat{\varphi}^{(s)}_{N,j}(t) \equiv 0 \); also, for any \( t > 0 \), \( \hat{\varphi}^{(s)}_{N,j}(t) \equiv 1_{\mathcal{D}_j} \). For any \( 1 \leq j < s \), any \( t > 0 \), and almost every \( Z_s \in \mathcal{D}_s \),

\[
0 \leq \hat{\varphi}^{(s)}_{N,j}(t, Z_s) \in (N - j)(N - j - 1)\ldots(N - s + 1)\mathbb{Z} \tag{35}
\]

**Proof.** Apply induction on \( s \). \( \square \)

**Proposition 5.3.** For any \( 1 \leq j < s \), any \( t > 0 \), and almost every \( Z_s \in \mathcal{D}_s \),

\[
0 \leq \hat{\varphi}^{(s)}_{N,j}(t, Z_s) \leq \prod_{j < k \leq s} \left( 4(N - k + 1) \left( 32k^2 \right)^{k^2} \right) \tag{36}
\]

**Proof.** Use induction on \( s \) and the collision bound from \([3]\). Note carefully that the spatial domain is \( \mathbb{R}^d \). \( \square \)

**Corollary 5.4.** For any \( 1 \leq j < s \), any \( t > 0 \), almost every point \( \tilde{Z}_s \in \mathcal{D}_s \) such that \( \hat{\varphi}^{(s)}_{N,j}(t, \tilde{Z}_s) \neq 0 \), and almost every \( Z_s \in \mathcal{D}_s \),

\[
0 \leq \hat{\varphi}^{(s)}_{N,j}(t, Z_s) \leq \hat{\varphi}^{(s)}_{N,j}(t, \tilde{Z}_s) \prod_{j < k \leq s} \left( 4 \left( 32k^2 \right)^{k^2} \right) \tag{37}
\]

**Proof.** Apply Lemma 5.2 and Proposition 5.3. \( \square \)

Motivated by Corollary 5.4 for \( 0 \leq k < s \) and \( T > 0 \), let us define

\[
\mathcal{W}_s^k(T) = \left\{ Z_s \in \mathcal{D}_s \mid \hat{\varphi}^{(s)}_{N,s-k}(T, Z_s) \neq 0 \right\} \tag{38}
\]

We have that \( \mathcal{W}_s^k(T_1) \subset \mathcal{W}_s^k(T_2) \) whenever \( 0 < T_1 < T_2 \).

**Proposition 5.5.** There exists a constant \( C_d > 0 \) such that the following is true: For any \( 0 < k < s \), any \( \beta > 0 \), and any \( T > 0 \), in the Boltzmann-Grad scaling \( N \sim k^{-1} = \ell^{-1} \), there holds

\[
\int_{\mathbb{R}^{2ds}} 1_{\mathcal{W}_s^k(T)} e^{-\beta(E_s(Z_s) + I_s(Z_s))} dZ_s \leq C(d, \beta)\ell^{-k} \frac{\prod_{q=0}^{k-1} (s - q)}{\prod_{q=1}^{k} (N - s + q)} \tag{39}
\]
**Proof.** The proof of Theorem 3.2 is easily adapted to apply to the functions $\tilde{\varphi}_{N,j}^{(s)}$, then we use Lemma 5.2.

**Remark.** Proposition 5.5 implies that, for any bounded set $B \subset \mathbb{R}^{2d_s}$, the set $B \cap \mathcal{W}_s^k(T)$ has measure of order $O(\epsilon^{k(d-1)})$; a similar result was found in [2].

**Proposition 5.6.** Consider the solution to the equations (29-30) with initial data

$$\hat{\varphi}_N^{(s)}(0, Z_s) = \begin{cases} N^k 1_{\mathcal{W}_s^k(T)} & \text{if } s = s_1 \\ 0 & \text{otherwise} \end{cases}$$

Then for a.e. $t > 0$, and a.e. $Z_s \in D_s$, we have

$$0 \leq \hat{\varphi}_N^{(s)}(t) \leq \begin{cases} 0 & \text{if } s < s_1 \\ C(K, s_1) N^{k+s-s_1} 1_{\mathcal{W}_s^{k+s-s_1}(T+t)} & \text{if } s_1 \leq s \leq K \\ \infty & \text{otherwise} \end{cases}$$

**Proof.** It is enough to observe that $\hat{\varphi}_N^{(s)}(0)$ is controlled from above (up to a constant depending on $s_1$) by $\hat{\varphi}_N^{(s)}(T)$, the same control from above is propagated to positive times, and then we can apply Proposition 5.3.

**Remark.** Proposition 5.6 shows that the sets $\mathcal{W}_s^k(T)$ are not artifacts of our choice of constant functions for the initial data. Indeed, even if we restart the dual BBGKY flow with a singular set as initial data, the further evolution is again concentrated on the same family of singular sets.

### 6. Observables and Pseudo-Trajectories

Pseudo-trajectories are fictitious trajectories which may be used to express the solution of the BBGKY hierarchy in terms of the initial data; they are a standard tool in the analysis of BBGKY-type hierarchies. [6, 11]

There is a close connection between observables and pseudo-trajectories; for instance, we can see by the fundamental duality relation (10) that observables allow us to express the solution of the BBGKY hierarchy in terms of the initial data. In some sense, we may view observables as a functional representation of pseudo-trajectories.

Recall that $\psi^s_t : D_s \to D_s$ denotes the flow of $s$ identical hard spheres of diameter $\epsilon$. We denote by $T_s(t)$ the operator which simply translates along trajectories:

$$\left( T_s(t) f^{(s)} \right)(Z_s) = f^{(s)} (\psi^{-1}_s Z_s)$$

The BBGKY hierarchy may be written in integral form using Duhamel’s formula:

$$f_N^{(s)}(t) = T_s(t) f_N^{(s)}(0) + (N - s) \epsilon^{d-1} \int_0^t T_s(t - t_1) C_{s+1} f_{N}^{(s+1)}(t_1) dt_1$$
A similar expression can be obtained for $f_N^{(s+1)}(t_1)$ and plugged into (43); this process can be repeated a finite number of times. Ultimately one is able to express any marginal $f_N^{(s)}(t)$ in terms of the initial data; that is,

$$f_N^{(s)}(t) = \sum_{k=0}^{N-s} a_{N,k,s} \int_0^t \cdots \int_0^{t_{k-1}} dt_k \cdots dt_1 \times$$

$$\times T_s(t-t_1)C_{s+1}T_{s+1}(t_1-t_2) \cdots C_{s+k}T_{s+k}(t_k)f_N^{(s+k)}(t_k)$$

(44)

where

$$a_{N,k,s} = \frac{(N-s)!}{(N-s-k)!} \varepsilon_k (d-1)^k$$

(45)

We will reformulate (44) using pseudo-trajectories. Pseudo-trajectories define a fictitious dynamics involving a variable number of particles. Let us be given $Z_s \in D_s$, a time $t > 0$, creation times $0 < t_k \leq \cdots \leq t_1 \leq t$, creation velocities $v_{s+j} \in \mathbb{R}^d$, impact parameters $\omega_j \in S^{d-1}$, and indices $i_j \in \{1, 2, \ldots, s+j-1\}$. The symbol

$$Z_{s,s+k} \left[ Z_s, t; \{ t_j, v_{s+j}, \omega_j, i_j \}_{j=1}^k \right]$$

(46)

means that we start with the given particles $Z_s$, and evolve backwards under the $s$ particle flow $\psi_s^t$ for a time $t-t_1$. Then we create a particle adjacent to the $i_1$ particle with velocity $v_1$ and impact parameter $\omega_1$, perform a collisional change of variables if needed, then continue the particle flow backwards for a time $t_1-t_2$, and so on. The end state, denoted by $Z_{s,s+k}[\ldots]$, is a configuration in $\mathbb{R}^{d(s+k)} \times \mathbb{R}^{d(s+k)}$. Associated with each pseudo-trajectory is an iterated collision kernel

$$b_{s,s+k} \left[ Z_s, t; \{ t_j, v_{s+j}, \omega_j, i_j \}_{j=1}^k \right]$$

(47)

Particle creations are usually referred to as collisions, whereas collisions induced by the dynamics (not creations) are usually called recollisions. We refer to [5, 6, 12] for precise definitions of pseudo-trajectories.

Remark. The pseudo-trajectory is not well-defined for impact parameters which would force particles to overlap at the time of particle creation.

We may now re-write (44) in the following form:

$$f_N^{(s)}(t, Z_s) = \sum_{k=0}^{N-s} a_{N,k,s} \times$$

$$\times \sum_{i_1=1}^{s} \cdots \sum_{i_k=1}^{s+k-1} \int_0^t \cdots \int_0^{t_{k-1}} \int_{\mathbb{R}^d} \int_{(S^{d-1})^k} \left( \prod_{m=1}^k d\omega_{i_m} dv_{s+m} dt_m \right) \times$$

$$\times \left( b_{s,s+k}[ \cdot ] f_N^{(s+k)}(0, Z_{s,s+k}[\cdot]) \right) \left[ Z_s, t; \{ t_j, v_{s+j}, \omega_j, i_j \}_{j=1}^k \right]$$

(48)
Let $E \subset D_s$ be a bounded measurable set which is symmetric under interchange of particle indices. Then we may write

\[
\int_{D_s} 1_{Z_s \in E} f_N^{(s)}(t, Z_s) dZ_s = \sum_{k=0}^{N-s} a_{N,k,s} \int_{D_s} dZ_s 1_{Z_s \in E} \times \\
\times \sum_{i_1=1}^{s} \cdots \sum_{i_k=1}^{s+k-1} \int_0^t \cdots \int_0^t \int_{\mathbb{R}^{dE}} \left( \prod_{m=1}^{k} d\omega_m dv_{s+m} dt_m \right) \times
\]

Using (15-16) we may now write

\[
\frac{1}{s!} \int_{D_s} 1_{Z_s \in E} f_N^{(s)}(t, Z_s) dZ_s = \sum_{k=0}^{N-s} \frac{1}{(s+k)!} \int_{D_{s+k}} \varphi_{N,E}^{(s+k)}(t, Z_{s+k}) f_N^{(s+k)}(0, Z_{s+k}) dZ_{s+k}
\]

Comparing (49) and (51), and recalling that $F_N(0)$ is an arbitrary sequence of symmetric functions, we conclude the following identity:

\[
\varphi_{N,E}^{(s+k)}(t, Z_{s+k}) = \sum_{\alpha} a_{N,k,s} b_{s,s+k}[Z_{s+k}^\alpha, t; \{t_j^\alpha, v_{s+j}^\alpha, \omega_j^\alpha, i_j^\alpha\}_{j=1}^k] \times \\
\times \left| \frac{\partial Z_{s,s+k} \left[ Z_{s+k}^\alpha, t; \{t_j^\alpha, v_{s+j}^\alpha, \omega_j^\alpha, i_j^\alpha\}_{j=1}^k \right]}{\partial Z_{s} \partial t_1 \cdots \partial t_k \partial v_{s+1} \cdots \partial v_{s+k} \partial \omega_1 \cdots \partial \omega_k} \right|^{-1}
\]

The (finite) sum $\sum_{\alpha}$ runs over all pseudo-trajectories which initially contain $s$ particles with $Z_{s+k}^\alpha \in E$, and end at a point (with $s+k$ particles) of the form $\sigma Z_{s+k}$ for some $\sigma \in S_{s+k}$\(^4\) Here $S_s$ is the symmetric group on $s$ letters which acts by interchange of particle indices; namely, $(\sigma Z_{s+1})_j = z_{\sigma(j)}$.

Comparing (52) with (17-18), we realize that each term appearing in the sum $\sum_{\alpha}$ in (52) is associated with a contribution to $\varphi_{N,E}^{(s+k)}$ equal to

\[
\pm (N-s-k+1)(N-s-k+2) \ldots (N-s)
\]

\(^4\)Note that two configurations $\sigma_1 Z_{s+k}$ and $\sigma_2 Z_{s+k}$ such that $\sigma_1^{-1} \sigma_2$ leaves fixed the last $k$ particle indices will correspond to physically indistinguishable collections of pseudo-trajectories. We do not double-count in this case.
Hence, in view of (55), we must have
\[
\begin{aligned}
&\left| \frac{\partial Z_{s,s+k}}{\partial Z_s \partial t_1 \ldots \partial t_k \partial v_{s+1} \ldots \partial v_{s+k} \partial \omega_1 \ldots \partial \omega_k} \right| \\
&\quad = \varepsilon^{k(d-1)} \left| b_{s,s+k} \left[ Z_s^\alpha, t; \left\{ t_j^\alpha, v_{s+j}^\alpha, \omega_j^\alpha, i_j^\alpha \right\}_{j=1}^k \right] \right| 
\end{aligned}
\] (54)

We remark that (54) appears in [13] as the result of a direct computation. The above argument supplies an alternative approach to deriving (54).

Finally we note that a formula similar to (52) is also available for the functions \( \varphi_{\Sigma,j}^{(s)} \) defined in Section (5). In particular, we easily deduce an alternative definition for the sets \( W_s^k(T) \). Let us define
\[
\mathcal{V}_s^k(T) = \left\{ Z_s \in \mathcal{D}_s \left| \begin{array}{l}
\exists Z_{s-k} \in \mathcal{D}_{s-k}, 0 < t_k < \cdots < t_1 < t < T, \\
v_{s+1}, \ldots, v_{s+k}, \omega_1, \ldots, \omega_k, i_1, \ldots, i_k, \\
such that \\
Z_s = Z_{s-k,s} \left[ Z_{s-k}, t; \{ t_j, v_{s+j}, \omega_j, i_j \}_{j=1}^k \right] 
\end{array} \right\} \right. \] (55)

Then we have
\[
W_s^k(T) = \bigcup_{\sigma \in \Sigma_s} \sigma \mathcal{V}_s^k(T) \] (56)

Notice that for any bounded set \( B \subset \mathbb{R}^{2d} \) which is symmetric under particle interchange, we have
\[
\left| B \cap \mathcal{V}_s^k(T) \right| \leq \left| B \cap W_s^k(T) \right| \leq (s+k)! \left| B \cap \mathcal{V}_s^k(T) \right| \] (57)

Hence the estimate from Proposition 5.5 (in particular the remark immediately following the proposition) applies equally well to either \( \mathcal{V}_s^k(T) \) or \( W_s^k(T) \).

7. Propagation of Chaos

We will require two auxiliary sets to state our main result. These sets appear in our proof for technical reasons and could actually be removed from the main theorem. Note that \( \eta > 0 \) is a small parameter which can depend on \( \varepsilon \).
\[
\mathcal{K}_s = \left\{ Z_s = (X_s, V_s) \in \mathcal{D}_s \left| \forall \tau > 0, \psi_s^{-\tau} Z_s = (X_s - V_s \tau, V_s) \right\} \right. \] (58)
\[
\mathcal{U}_s^0 = \left\{ Z_s \in \mathcal{D}_s \left| \inf_{1 \leq i < j \leq s} |v_i - v_j| > \eta \right\} \right. \] (59)

Using the sets defined above, we introduce an \( L^1 \) seminorm defined as follows:
\[
\left\| f^{(s)} \right\|_{L^1_{Z_s \cap \mathcal{U}_s^0 \cap \mathcal{V}_s^k(T)}(\varepsilon, s, k, \eta, T', R)} = \varepsilon^{-k(d-1)} \left\| f^{(s)} \chi_{\mathcal{K}_s \cap \mathcal{U}_s^0 \cap \mathcal{V}_s^k(T)}(\varepsilon, s, k, \eta, T')(Z_s) \right\|_{L^1_{Z_s}} \] (60)
Finally, we assume there exists a decreasing sequence of open balls that we furthermore assume that there exists some \( f \) which satisfy the conditions of Theorem 7.1, but which do not converge uniformly as required by Lanford’s original proof. \([11]\) We begin with a 7.1. An Example. We are going to construct sequences of initial data (\( s, k, \eta, T, R \)) such that

\[
\sup_{0 \leq t \leq T} \sup_{x \in \mathbb{R}^d} \sup_{v \in \mathbb{R}^d} e^{\frac{1}{2} \beta_0 |v|^2} f(t, x, v) < \infty
\]

and \( f(t) \in W^{1, \infty}(\mathbb{R}^d \times \mathbb{R}^d) \) for \( t \in [0, T] \). Let \( f_N(0) \) be a symmetric probability density on \( D_N \) for each \( N \in \mathbb{N} \), and enforce the Boltzmann-Grad scaling \( N \varepsilon^{-d-1} = \ell^{-1} \). Suppose that there exists a \( \beta_T > 0 \), \( \mu_T \in \mathbb{R} \) such that the marginals \( f_N^{(s)} \) of \( f_N \) satisfy

\[
\sup_{0 \leq t \leq T} \sup_{s \leq N} \sup_{Z_i \in D_s} e^{\beta_T E_s(Z_s)} e^{\mu_T s} \left| f_N^{(s)}(t, Z_s) \right| < \infty
\]

Let \( \eta(\varepsilon) = \sqrt{\varepsilon} \). Assume that for all \( s \in \mathbb{N} \), \( 0 \leq k < s \), \( T' > 0 \), and \( R > 0 \), we have

\[
\lim_{N \to \infty} \left\| \frac{f_N^{(s)}(0)}{\varepsilon, s, k, \eta(\varepsilon), T', R} - f(0) \right\| = 0
\]

Then for all \( s \in \mathbb{N} \), \( 0 \leq k < s \), \( T' > 0 \), \( R > 0 \), and \( t \in [0, T] \), we have

\[
\lim_{N \to \infty} \left\| \frac{f_N^{(s)}(t)}{\varepsilon, s, k, \eta(\varepsilon), T', R} - f(t) \right\| = 0
\]

7.1. An Example. We are going to construct sequences of initial data which satisfy the conditions of Theorem 7.1 but which do not converge uniformly as required by Lanford’s original proof. \([11]\) We begin with a sequence of functions \( 0 \leq f_{0,N} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) such that, for some \( \beta_0 > 0 \),

\[
\sup_{N \in \mathbb{N}} \sup_{x \in \mathbb{R}^d} \sup_{v \in \mathbb{R}^d} e^{\frac{1}{2} \beta_0 (|x|^2 + |v|^2)} f_{0,N}(x, v) < \infty
\]

We also assume

\[
\int_{\mathbb{R}^d \times \mathbb{R}^d} f_{0,N}(x, v) dx dv = 1
\]

We furthermore assume that there exists some \( f_0 \) in the Schwartz class such that

\[
\lim_{N \to \infty} \| f_{0,N} - f_0 \|_{L_v^1} = 0
\]

Finally, we assume there exists a decreasing sequence of open balls \( B_N \subset \mathbb{R}^d \times \mathbb{R}^d \) such that \( \bigcap_N B_N = \emptyset \) and

\[
\lim_{N \to \infty} \inf_{(x,v) \in B_N} \left( f_{0,N}(x,v) - f_0(x,v) \right) > 0
\]
We also assume that the Lebesgue measure of $B_N$ is at least $C(\log N)^{-1}$ for some constant $C$.

The $N$-particle data is then defined as
\[
 f_N(Z_N) = Z_N^{-1} f_{0,N}^\otimes(Z_N) 1_{Z_N \in D_N} \tag{69}
\]
where
\[
 Z_N = \int f_{0,N}^\otimes(Z_N) 1_{Z_N \in D_N} dZ_N \tag{70}
\]
is a normalization factor. In the Boltzmann-Grad scaling (See [6] or [5] for a proof.) The functions $f$ are assumed to be normalized by $D_N$.

We also assume that the Lebesgue measure of $B$ is possible to show that for all $s \in \mathbb{N}$ there holds:
\[
 \limsup_{N \to \infty} \left\| 1_{Z_s \in D_s} \left( f_N^{(s)}(0, Z_s) - f_{0,N}^\otimes(Z_s) \right) \right\|_{L^\infty_{Z_s}} = 0 \tag{71}
\]
(See [6] or [5] for a proof.) The functions $f_{0,N}$ do not converge uniformly on compact sets, so by (71), the functions $f_N^{(s)}(0)$ also do not converge uniformly on compact sets. Therefore the hypotheses of Lanford’s theorem are not fulfilled.

We are going to show that the conditions of Theorem [7,1] are satisfied, using the triangle inequality. Indeed, for any $Z_s \in D_s$, we have
\[
 f_N^{(s)}(0, Z_s) - f_{0,N}^\otimes(Z_s) \leq \left| f_N^{(s)}(0, Z_s) - f_{0,0}^\otimes(Z_s) \right| + \\
 \sum_{i=1}^s f_{0,N}^\otimes(Z_s) \left| f_{0,N}(z_i) - f_0(z_i) \right| \tag{72}
\]

The first term on the right hand side of (72) is estimated using (71) and the bound
\[
 \left\| f^{(s)} \right\|_{\infty, s, k, \eta, T', R} \leq C(s, k, T', R) \left\| f^{(s)} \right\|_{\infty} \tag{73}
\]
The remaining terms are all estimated in the same way so we only consider the case $i = 1$. We are trying to bound
\[
 \left\| f_{0,N}(z_1) - f_0(z_1) \left| f_0^\otimes(Z_2, s) \right| \right\|_{\infty, s, k, \eta, T', R} \tag{74}
\]
Since $f_0 \leq Ce^{-\frac{1}{2} \beta_0(|x|^2 + |v|^2)}$, we are left with
\[
 C^s \left\| f_{0,N}(z_1) - f_0(z_1) \right\| e^{-\beta_0(E_{s-1}+I_{s-1})} \left\| f_0^\otimes(Z_2, s) \right\|_{\infty, s, k, \eta, T', R} \tag{75}
\]
Now the point is that the condition $Z_s \in V^k(T')$ can be interpreted as saying that $z_1$ is chosen arbitrarily, and then the $k$ collision constraints are simply constraints imposed on the remaining particles. Since we have an $L^\infty$ bound in all but the first coordinate, we gain a factor of $\varepsilon^{d-1}$ for each of the $k$ collision constraints, so that
\[
 \left\| f_{0,N}(z_1) - f_0(z_1) \right\| e^{-\beta_0(E_{s-1}+I_{s-1})} \left\| f_0^\otimes(Z_2, s) \right\|_{\infty, s, k, \eta, T', R} \leq \\
 \leq C(s, k, T', R) \left\| f_{0,N} - f_0 \right\|_{L^1_{x,v}} \tag{76}
\]
which yields the desired bound.

**Remark.** Note that the conclusion of Theorem 7.1 implies that the first marginal $\mathcal{F}_{\rho}^{(1)}(t)$ converges to $f(t)$ in the norm topology of $L^1_{x,v}$. Similarly, as the example illustrates, the hypotheses of the theorem are related to $L^1$ convergence of the first marginal at $t = 0$. Hence, Theorem 7.1 provides a microscopic interpretation for $L^1$ convergence in the Boltzmann-Grad limit.

### 7.2. Proof of Theorem 7.1

Following [5], we may assume that, for some $\beta_0 > 0$, $\mu_0 \in \mathbb{R}$, there holds

\[
\sup_{1 \leq s \leq N} \sup_{Z_s \in D_s} \left| J_{N}^{(s)}(0, Z_s) \right| e^{\beta_0(E_s + I_d)(Z_s)} e^{|\mu_0 s|} \leq 1
\]

(77)

The following error estimate was proven on a small time interval $[0, T_L]$, using suitable truncations in $L^\infty$: (see [5] for details)

\[
\left| \left( f_{N}^{(s)} - f^{\otimes s} \right)(t, Z_s) \right| 1_{Z_s \in K_s \cap \mathcal{U}_d^s} 1_{(E_s + I_d)(Z_s) \leq 2R^2} \leq 3e^{-(\mu_0 - 2)s} e^{|\beta_0 R^2| + e^{-n}} + \\
+ \left[ 1 - \left( 1 - \frac{n}{N} \right)^n \right] e^{-\mu_0 s} e^{C_d \ell^{-1} n R^{d+1} e^{-\mu_0 T_L}} + \\
+ 2e^{-\mu_0 s} n^2 A_{\eta R} \left[ \alpha + \frac{y}{\eta T_L} + C_{d,\alpha} \left( \frac{\eta}{R} \right)^{d-1} + C_{d,\alpha} \theta^{(d-1)/2} \right] + \\
+ C_{d,\alpha} e^{C_d \ell^{-1} n R^{d+1} e^{-\mu_0 T_L}} + \\
+ C_{d,\alpha} e^{C_d \ell^{-1} n R^{d+1} e^{-\mu_0 T_L}} \sup_{1 \leq j \leq n} \left| \nabla Z_j \left( f^{\otimes j} \right)(0, Z_j) \right| 1_{(E_j + I_j)(Z_j) \leq 2R^2} + \\
+ C_{d,\alpha} e^{C_d \ell^{-1} n R^{d+1} e^{-\mu_0 T_L}} \times \\
\times \sup_{1 \leq j \leq n} \left| J_{N}^{(j)} - f^{\otimes j} \right| 1_{Z_j \in K_j \cap \mathcal{U}_d^j} 1_{(E_j + I_j)(Z_j) \leq 2R^2}
\]

(79)

We care only about the last term, $VI$, which is (ignoring the prefactor):

\[
\sup_{1 \leq j \leq n} \left| J_{N}^{(j)} - f^{\otimes j} \right| 1_{Z_j \in K_j \cap \mathcal{U}_d^j} 1_{(E_j + I_j)(Z_j) \leq 2R^2}
\]

(80)
It is this last term which we desire to estimate in $L^1$ instead of $L^\infty$. From the proof of [5], we are free to replace $VI$ in (79) by $VI'$ where

$$VI' =$$

$$= \sum_{j=0}^{n-s} \sum_{i_1=1}^{s} \cdots \sum_{i_{j}=1}^{s+j-1} \ell^{-j} \int_0^t \cdots \int_0^{t_{j-1}} \int_{(B_{2R}^j)^j} \prod_{m=1}^{j} dw_m dv_{s+m} dt_m \times$$

$$\times (1 - 1_{B_j}) \times$$

$$\times \left| b_{s,s+j}^{(1)} \right| \left| 1_{(E_{s+j} + I_{s+j})(Z_{s,s+j}[^{\cdot}])} \leq 2R^2 \right| \times$$

$$\times \left| f_N^{(s+j)}(0, Z_{s,s+j}[^{\cdot}]) - f^{(s+j)}(0, Z_{s,s+j}[^{\cdot}]) \right| \left| Z_s, t; \{t_r, v_{s+r}, \omega_r, i_r\}_{r=1}^{j} \right|$$

(81)

The set $B_j$ specifies a “bad set” of particle creations which may lead to recollisions. In particular, $Z_{s,s+j}[^{\cdot}]$ is in $K_{s+j} \cap U_{s+j}^0$.

Recall that

$$\left\| f^{(s)} \right\|_{\varepsilon,s,k,\eta,T',R} \leq C(s,k,T',R) \left\| f^{(s)} \right\|_{\infty}$$

(82)

so the terms $I$ through $V$ in (79) are disposed with easily. We only have to estimate

$$\left\| VI' \right\|_{\varepsilon,s,k,\eta,T',R}$$

(83)

We can do that, in fact, because pseudo-trajectories obey a determinant identity (see [5] or [13]):

$$\left| \det \frac{\partial Z_{s,s+j}[Z_s, t; \{t_r, v_{s+r}, \omega_r, i_r\}_{r=1}^{j}]}{\partial Z_s \partial t_1 \cdots \partial t_j \partial v_{s+1} \cdots \partial v_{s+j} \partial \omega_1 \cdots \partial \omega_j} \right| =$$

$$= \varepsilon^{(d-1)} \left| b_{s,s+j}[Z_s, t; \{t_r, v_{s+r}, \omega_r, i_r\}_{r=1}^{j}] \right|$$

(84)

Each additional collision integral in (81) brings down an extra power of $\varepsilon^{-(d-1)}$ according to (84), but this is exactly compensated by an extra $\varepsilon^{d-1}$ coming from the definition of the norm $\left\| f^{(s+j)} \right\|_{\varepsilon,s+j,k,j,\eta,T',R'}$. This is because particle creation maps $V_{s+j}^{k+j}(T')$ to $V_{s+j+1}^{k+j+1}(T')$. In fact the only difficulty is that the map $Z_{s,s+k}[\cdots]$ is not injective, but the lack of injectivity can be quantified since there are no recollisions for any pseudo-trajectory appearing in our estimate (at least along the time interval of interest).

Altogether we can write (up to combinatorial constants)

$$\left\| VI' \right\|_{\varepsilon,s,k,\eta,T'-t,R} \leq \sum_{j=0}^{n-s} \left\| f_N^{(s+j)}(0) - f^{(s+j)}(0) \right\|_{\varepsilon,s+j,k+j,\eta,T',R}$$

(85)

which tends to zero as $N \to \infty$, by assumption. Taking limits as in [5], we are able to conclude.


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