Boltzmann-Grad Limit for Hard Sphere Model

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1 Introduction

Boltzmann's groundbreaking work on the kinetic theory of gases revolutionized thermodynamics, and led to the creation of statistical mechanics. In 1872 Boltzmann proposed an integro-differential equation to describe the evolution of the particle density of a rarefied gas. In his celebrated H-Theorem, Boltzmann verified the second law of thermodynamics for his equation, and confirmed Maxwell's statistical model of equilibrium states.

In 1900, Hilbert published 23 problems that helped set the mathematics research agenda in the 20th century. Hilbert's sixth problem was motivated by Boltzmann's work on the kinetic theory of gases. Microscopically a gas is modeled by a large collection of particles that are interacting according to Newton's law. Boltzmann's mesoscopic description involves a particle density that solves a nonlinear partial differential equation. Macroscopically a gas or fluid is governed by Euler and Navier-Stokes equations.

In his sixth's problem, Hilbert asked the question of giving a mathematically rigorous derivation for the macroscopic equations of fluids, from the Newtonian laws governing microscopic particle dynamics. In other words, Hilbert proposed a unified theory for gas/fluid dynamics that includes three levels of descriptions: microscopic, mesoscopic and macroscopic. Hilbert's sixth problem consists of two steps:

1. (Kinetic Limit) The derivation of Boltzmann's kinetic equation from the microscopic Newtonian dynamics of a rarefied gas.

2. (Hydrodynamic Limit) The derivation of the fluid equations from Boltzmann's kinetic equation as collision rates goes to infinity (equivalently, as the gas gets denser).

The hydrodynamic limit for the Boltzmann equation leading to incompressible fluid equations is rather well-understood, as a result of series of progresses that were made by many authors during the last decade of the 20th century.

The precise mathematical formulation of the kinetic limit was given by Grad in 1949. In reality the number of particles is given by the Avogadro number and the effective interparticle interaction is microscopically small. To derive Boltzmann equation from such a large interacting particle system, we need to apply some kind of "law of large numbers" by sending the number of particles N to infinity, and sending the interaction distance ϵ to zero. For the validity of the Boltzmann equation, we need to make sure that a typical particle interact with finitely many particles in one unit of time. For this to be the case, Grad discovered that N must be related to ϵ by $N \sim \epsilon^{d-1}$, where d is the spatial dimension.

Boltzmann's derivation of his kinetic equation was based on his *Stosszahlansatz (molecular chaos hypothesis)*. More precisely, if initially particles of a gas are statistically independent, the correlations built at later times are negligible, and can be ignored. The rigorous verification of this hypothesis is the main challenge in the derivation of Boltzmann equation.

The first breakthrough in the kinetic limit part of Hilbert's sixth problem was achieved by Lanford in 1975. He showed that Boltzmann equation does indeed approximate the particle density in large N limit provided that Grad's relationship holds, and time is sufficiently short.

Recently,Yu Deng, Zaher Hani, and Xiao Ma have settled the long-time derivation of the Boltzmann equation from a hard sphere system provided that the Boltzmann equation possesses a classical solution.

In Hilbert's sixth problem, the microscopic description of a gas was governed by the Newtonian mechanics. With the discovery of quantum mechanics, Boltzmann's kinetic theory of rarefied gases had to be revised. Kinetic equations are widely used to understand dynamical aspects of quantum many particle systems. In a mean field regime, the Schrodinger equation of large number of bosanic particles can be approximated with the non-linear Schrodinger equation.

1.1 Hard Sphere Model (HSM)

Microscopically a gas is modeled by a Hamiltonian ODE in $\mathbb{R}^{2d}$. A gas of N particles is described by a vector $\mathbf{q} = (\mathbf{x}, \mathbf{v})$, where $\mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{dN}$ denotes the location of particles in $\mathbb{R}^d$, and $\mathbf{v} = (v_1, \ldots, v_N) \in \mathbb{R}^{dN}$ denotes the velocity of particles. By Newton's equation

$$\begin{aligned} \frac{dx_i}{dt} &= v_i \\ \frac{dv_i}{dt} &= -\sum_{j\neq i} \nabla V(x_i - x_j) \qquad\qquad i, j = 1, 2, \ldots, N \end{aligned}$$

where V represents the potential governing the two-body interaction between particles. Assuming $V(z) = W(|z|)$ is radially symmetric (i.e., the force in central) leads to the conservation of momentum, energy and angular momentum. That is

$$\frac{d}{dt}\sum_i v_i = 0,$$
$$\frac{d}{dt}\sum_i x_i \times v_i = 0,$$
$$\frac{d}{dt}\left\{\frac{1}{2}\sum_i |v_i|^2 + \sum_{i\neq j} V(x_i - x_j)\right\} = 0.$$

(For the conservation of angular momentum in dimension $d > 3$ we replace the vector $x \times v$ with the matrix $(x^i v^j - x^j v^i : 1 \le i, j \le d)$.) If the gas is dilute, then $N \ll \varepsilon^{-d}$ where N is the total number of particles and ε is the diameter of each particle. For our purposes we assume that $V(z) = V^\varepsilon(z) = W\left(\frac{|z|}{\varepsilon}\right)$ with W a function of compact support, so that the range of interaction is of order $O(\varepsilon)$. To have a more manageable situation, we consider an extreme case of the above scenario, namely when

$$W(r) = \begin{cases} \infty & \text{if } |r| \le 1, \\ 0 & \text{if } r > 1. \end{cases} \tag{1.1}$$

For this case, we have a simple description of our model. The potential (1.1) prevents a pair of particles to have a distance less than ε. This means that so long as $|x_i - x_j| > \varepsilon$, the potential energy is zero. In summary, we always have $|x_i - x_j| \ge \varepsilon$ for $i \ne j$ and $\frac{dx_i}{dt} = v_i$, $\frac{dv_i}{dt} = 0$ whenever $|x_i - x_j| > \varepsilon$, i.e., each particle travels according to its velocity except when two particles collide. At a collision, the pre-collisional velocities (v_i, v_j) change to post-collisional velocities (v_i^j, v_j^i). To figure out what (v_i^j, v_j^i) is, recall that our system enjoys three conservation laws: the conservation of momentum, angular momentum and energy. More precisely,

$$v_i^j + v_j^i = v_i + v_j, \quad |v_i^j|^2 + |v_j^i|^2 = |v_i|^2 + |v_j|^2, \quad v_i^j \times x_i + v_j^i \times x_j = v_i \times x_i + v_j \times x_j.$$

By the conservation of momentum and energy,

$$v_i^j = v_i + a, \;\; v_j^i = v_j - a,$$

for $a = (v_j - v_i) \cdot n\, n$ for a unit vector n. The conservation of angular momentum forces $n = n_{ij} = \frac{x_i - x_j}{|x_i - x_j|}$. In summary, the n_{ij}-component of v_i and v_j are interchanged:

$$v_i^j = v_i - (v_i - v_j) \cdot n_{ij} n_{ij}, \quad n_{ij} = \frac{x_i - x_j}{|x_i - x_j|}. \tag{1.2}$$

Boltzmann derived an important PDE for the evolution of the macroscopic densities in the case of a dilute gas. To describe this derivation, we need to be more precise about the assumption $N \ll \varepsilon^{-d}$. In 1949 Grad discovered that indeed one needs $N = O(\varepsilon^{1-d})$ for the Boltzmann derivation. In fact, Boltzmann derivation was based on several assumptions. The first assumption says that the mean free path of a particle in a dilute gas is positive and finite. The mean free path is the time a typical particle travels in average with no collision encounter. Note that each particle is a sphere of diameter ε. Such a particle traces a set of volume $O(\varepsilon^{1-d})$ in one unit of time. If particles are scattered evenly in space, we find $O(N\varepsilon^{1-d})$ many particles in a set of volume $O(\varepsilon^{1-d})$. Hence typically a particle encounters finitely many particles in one unit of time. This can be rephrased as the positiveness of the mean free path.

1.2 Kinetic Limit

As we mentioned previously, for a dilute gase, we assume that $N = O(\varepsilon^{1-d})$, for a constant $\lambda > 0$. This guarantees finiteness and positivity of the mean free path of the gas. Boltzmann's equation yields a mesoscopic equation for the evolution of the particle densities. By a density we mean a function $f(x, v, t)$ such that

$$\varepsilon^{d-1} \sum_{i=1}^{N} \zeta(x_i(t), v_i(t)) \to \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \zeta(x, v) f(x, v, t) dx dv \tag{1.3}$$

for every bound continuous function ζ. Normally we assume (1.3) is valid initially for a function $f(x, v, 0) = f^0(x, v)$, and expect to have (1.3) at later times for a suitable function $f(x, v, t)$. Note carefully that if (1.3) is valid at $t = 0$, then

$$\lim_{\varepsilon \to 0} \varepsilon^{d-1} N = Z := \iint f^0(x, v) dx dv.$$

Boltzmann was the first who derived a PDE from the evolution of the density f in the case of HSM. According to Boltzmann, f must satisfy

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} = Q(f) := Q^+(f) - Q^-(f), \tag{1.4}$$

where $Q^-(f) = f\mathcal{L}f$, with

$$\mathcal{L}f(v) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} B(v - v_*, n) f(x, v_*, t) \; dn dv_*, \tag{1.5}$$

with $B(v - v_*, n) = [(v - v_*) \cdot n]^+$, and

$$Q^+(f, f) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} B(v - v_*, n) f(x, v', t) f(x, v'_*, t) dn dv_*. \tag{1.6}$$

Here, dn represents the standard surface measure on the unit sphere, and

$$\begin{aligned} v' &= v - (v - v_*) \cdot n \, n, \\ v_*' &= v + (v - v_*) \cdot n \, n. \end{aligned}$$

The term $B(v-v_*, n)f(x, v, t)f(x, v_*, t)$ represents the *loss term*. Its form has to do with the celebrated *molecular chaos* assumption of Boltzmann. This assumption roughly asserts that before a collision, particles are (approximately) stochastically independent. Hence the probability of having a pair of particles near a point x at time t, with velocities v and v_*, is approximately $f(x, v, t)f(x, v_*, t)$. The *gain term* has a similar interpretation.

In the case of the HSM, the initial condition (1.3) holds if the particle configurations $\mathbf{q} = (x_1, v_1, \ldots, x_N, v_N)$ is selected randomly according to the measure

$$\frac{1}{Z_N} f^0(x_1, v_1) f^0(x_2, v_2) \ldots f^0(x_N, v_N) \; dx_1 dv_1 \ldots dx_N dv_N \tag{1.7}$$

with

$$Z_N = \int \cdots \int f^0(x_1, v_1) \ldots f^0(x_N, v_N) \mathbb{1}(\mathbf{q} \in \Omega) \; dx_1 dv_1 \ldots dx_N dv_N$$

where

$$\Omega = \{\mathbf{q} : |x_i - x_j| > \varepsilon \text{ for all } i \neq j\}.$$

We are now ready to state part of Hilbert's sixth problem:

Conjecture 1.1 Take a function $f^0 \geq 0$ with $\int f^0 dx dv < \infty$. Assume that $\mathbf{q}$ is initially distributed according to (1.7). Then (1.3) holds for all t, where f is the unique solution to the Boltzmann equation (1.4), subject to the initial condition $f(x, v, 0) = f^0(x, v)$. □

Lanford in 1975 established Conjecture 2.1 for short times:

Theorem 1.1. *There exists $t_0 = t_0(f^0) > 0$ such that the Conjecture* 1.1 *is valid for $t < t_0(f^0)$.*

Lanford's method [La] is perturbative and is based on the BBGKY hierarchy equations.

The main challenge in studying Boltzmann's equation stems from the quadratic form of Q. We may regard (1.4) as an ODE in infinite dimension. Recall that the ODE $\frac{dx}{dt} = x^2$ does not have a global solution in t. We expect PDE (1.4) to be well-posed because of the special structure of Q, in particular the subtle cancellation in $Q = Q^+ - Q^-$. However, Lanford's method does not take advantage of this cancellation, and is not expected to work globally in time.

Illner and Pulvirenti [IP], using a similar idea replaces the smallness in time with the smallness in the initial data:

Theorem 1.2. *There exists a constant $C(\beta)$ such that if*

$$f^0(x,v) \leq C(\beta)\exp(-\beta(|x|^2+|v|^2))),$$

then the Conjecture 1.1 *holds for all times.*

The issue of existence and uniqueness of solutions to Boltzmann's equation is not well-understood. DiPerna and Lions [DLi] established the existence of a so-called *renormalized* solution in 1985. The uniqueness of the renormalized solution remains open. However, Lions [Li] shows that if there exists a bounded solution to (1.4), then the renormalized solution is unique. The existence of a bounded solution for any bounded f^0 is a long-standing open problem. The main challenge is as how to control the collision terms $Q^{\pm}$. It is an open problem to show $\int_0^T \iint Q^{\pm} dxdvdt < \infty$. Microscopically this corresponds to showing that in average N^{-1} times the total number of collision encounters occurring in a time interval $[0,T]$ is finite. This is just the first step in establishing Conjecture 1.1. Moreover, we need to verify some variant of the Stosszahlensatz (molecular chaos hypothesis) of Boltzmann. Lanford's interpretation of this principle is this: If initially the probability density of the configuration is given by a product like (1.7), then this property is almost true at later times as N gets large. A different interpretation of Stosszahlensatz is given in [R1] and [R2].

1.3 Boltzmann H-Theorem and Renormalized Solutions

When $d \geq 2$, the best existence result available for (1.4) is due to DiPerna and Lions [DLi1]. This existence result is formulated for the so-called renormalized solutions and the uniqueness for such solutions is an open problem. Note however that if we already know a bounded strong solution exists, then there exists a unique renormalized solution [Li]. Before we give a precise definition of a renormalized solutions, we discuss some of existing estimates for solutions.

We first describes the conservation laws. Assume that the collision kernel B satisfies

$$B(v,n) = B(-v,-n), \quad B(v - 2v\cdot nn, n) = B(v,n),$$

so that the following physically natural identities hold

$$B(v-v_*,n) = B(v_*-v,-n), \quad B(v'-v'_*,n) = B(v-v_*,n). \tag{1.8}$$

We also use the compact notation $f_* = f(v_*)$, $f' = f(v')$, and $f'_* = f(v'_*)$.

Observe that if $\psi : \mathbb{R}^d \to \mathbb{R}$ is a bounded continuous function, and

$$U(x,t;\psi) = \int \psi(v) f(x,v,t)\ dv, \quad V(x,t;\psi) = \int v\psi(v) f(x,v,t)\ dv,$$

then by (1.8),

$$U_t + v \cdot V_x = \frac{1}{2} \iint \int_{\mathbb{S}^{d-1}} B(v - v_*, n) f f_* \big(\psi(v') + \psi(v'_*) - \psi(v) - \psi(v_*)\big) \; dv dv_* dn. \tag{1.9}$$

This yields $d + 2$ many conservation laws by choosing $\psi \in \{1, v, |v|^2$. Indeed if

$$\begin{aligned} &\rho(x,t) = U(x,t;1), \quad (\rho u)(x,t) = U(x,t;v), \quad 2(\rho E)(x,t) = U(x,t;|v|^2), \\ &A(x,t) = U(x,t; v \otimes v), \quad 2B(x,t) = U(x,t;|v|^2 v) \end{aligned}$$

then we have

$$\begin{aligned} &\rho_t + \nabla \cdot (\rho u) = 0, \\ &(\rho u)_t + \nabla A = 0, \\ &(\rho E)_t + \nabla \cdot B = 0. \end{aligned} \tag{1.10}$$

In particular,

$$\frac{d}{dt} \int \rho(x,t) \; dx = 0, \quad \frac{d}{dt} \int (\rho u)(x,t) \; dx = 0, \quad \frac{d}{dt} \int (\rho E)(x,t) \; dx. \tag{1.11}$$

Similarly, we set

$$\mathcal{H}(f)(x,t) = \int f(x,v,t) \log f(x,v,t) \; dv, \quad \mathcal{R}(f)(x,t) = \int v f(x,v,t) \log f(x,v,t) \; dv,$$

which is as if we choose $\psi = \log f$ in (1.9) (in spite of dependence on (x,t). As in (1.9), we can readily show

$$\mathcal{H}(f)_t + \nabla \cdot \mathcal{R}(f) = -\mathcal{E}(f), \tag{1.12}$$

where

$$\begin{aligned} \mathcal{E}(f) &= -\int Q(f)(\log f + 1) \; dv = -\int Q(f) \log f \; dv \\ &= -\frac{1}{2} \iint \int_{\mathbb{S}^{d-1}} B(v - v_*, n) f f_* \log \frac{f' f'_*}{f f_*} \; dv dv_* dn \\ &= \frac{1}{4} \iint \int_{\mathbb{S}^{d-1}} B(v - v_*, n)(f' f'_* - f f_*) \log \frac{f' f'_*}{f f_*} \; dv dv_* dn \geq 0. \end{aligned}$$

Let us set

$$H(f)(t) = \int \mathcal{H}(f)(x,t) \; dx.$$

From (1.11) we deduce the following important bounds: f solves (1.4) in the time interval $[0,T]$, then

$$\sup_{t\in[0,T]} H(f)(t) \leq H(f)(0), \qquad \int_0^T \int \mathcal{E}(f)(x,t)\ dxdt \leq H(f)(0). \tag{1.13}$$

The entropy equation (1.12) can be used to determine spatially homogeneous equilibrium states. More precisely, if $f(x,v,t) = M(v)$ solves (1.4), then by (1.12), we must have $\mathcal{E}(M) = 0$. This is equivalent to saying that $MM_* = M'M'_*$ for every $v, v_* \in \mathbb{R}^d$ and $n \in \mathbb{S}^{d-1}$. If $\log M = h$, then h satisfies the conservation law

$$h(v') + h(v'_*) = h(v) + h(v_*). \tag{1.14}$$

Let us write $\mathcal{C}$ for the set of continuous functions $h : \mathbb{R}^d \to \mathbb{R}$ for which (1.14) holds for every $v, v_* \in \mathbb{R}^d$ and $n \in \mathbb{S}^{d-1}$. It was shown by Boltzmann that $\dim \mathcal{C} = d+2$, and that $\mathcal{C}$ is spanned by $1, v$, and $|v|^2$. In this way Boltzmann has shown that his equation is consistent with the Maxwell statistical equilibrium model of gases. More precisely, an equilibrium solution M can be represented as

$$M(v) = M_{\rho,u,\theta}(v) = \rho(2\pi R\theta)^{-d/2}\ e^{-\frac{|v-u|^2}{2\theta R}}, \tag{1.15}$$

for a constant $(\rho, u, \theta) \in (0,\infty) \times \mathbb{R}^d \times (0,\infty)$. Observe

$$\rho = \int M(v)\ dv, \qquad \rho u = \int vM(v)\ dv, \qquad \rho E = \rho\left(\frac{1}{2}|u|^2 + e\right) = \int \frac{1}{2}|v|^2\ dv, \tag{1.16}$$

for $e = dR\theta/2$. The solution M given by (1.15) is known as a Maxwellian, modeling an *ideal gas* at equilibrium. The constants ρ, u, e, and R represent the mass, the momentum, the internal energy, and the gas constant. We are now ready to explain the hydrodynamic limit part of the Hilbert's sixth problem: If f^κ solves

$$f^\kappa_t + v \cdot f^\kappa_x = \kappa^{-1} Q(f^\kappa), \tag{1.17}$$

with κ representing the *Knudsen number*, then as $\kappa \to 0$, the solution f^κ is approximating a local Maxwellian of the form $M_{\rho(x,t),u(x,t),\theta(x,t)} := M(x,t)$. If we substitute $M(x,t)$ for $f = f^\kappa$ in (1.10), we are led to the Euler (hydrodynamic) equation:

$$\begin{aligned} &\rho_t + \nabla \cdot (\rho u) = 0, \\ &(\rho u)_t + \nabla\big(\rho(u \otimes u)\big) + \nabla p = 0, \\ &(\rho E)_t + \nabla \cdot \big((\rho E + p)u\big) = 0, \end{aligned} \tag{1.18}$$

where the pressure p is given by $p = R\rho\theta$.

As the first attempt, we may consider weak solutions to (1.4). To make sense of a weak solution, we need to make sense of $\int Q^{\pm}(f)\zeta\ dxdvdt$, for a test function ζ of compact support. This is well-defined if $Q^{\pm}(f)\in L^1_{loc}$. Our conservation laws and (1.13) are not strong enough to accommodate a local L^1 bounds on $Q^{\pm}$. The following definition proposes a notion of a solution that avoids L^1 bounds on collision terms.

Definition 1.1 We say that f is a *renormalized solution* of (1.4) if

$$f\in L^1([0,\infty)\times\mathbb{T}^d\times\mathbb{R}^d),\quad f\geq 0\ ,\quad \frac{Q^{\pm}(f)}{1+f}\in L^1([0,T]\times\mathbb{T}^d\times\mathbb{R}^d)\ ,$$

for every positive T, and for every Lipschitz continuous $\beta:[0,\infty)\to\mathbb{R}$ that satisfies

$$\sup_r (1+r)|\beta'(r)|<\infty\ ,$$

we have that

$$\beta(f)_t+v\dot{\beta}(f)_x=\beta'(f)Q(f,f)$$

in weak sense. □

An important aspect of the Boltzmann equation is the smoothing effect of its flow term $\partial_t+v\cdot\partial_x$. This is known as the velocity averaging lemma and was quantitatively formulated and studied by Glose et al. in [GLiPS]. The velocity averaging lemma has the following flavor: If both f and $\frac{\partial f}{\partial t}+v\cdot\frac{\partial f}{\partial x}$ belong to a weakly compact subset of $L^1(\mathbb{T}^d\times\mathbb{R}^d\times[0,T])$ and ψ is a bounded smooth function, then the velocity average $\int f(x,v,t)\psi(v)dv=:\rho(x,t)$ belongs to a strongly compact subset of $L^1(\mathbb{T}^d\times\mathbb{R}^d\times[0,T])$. More concretely, if $f_t+v\cdot f_x=g$, and $\rho(x,t)=U(x,t;\psi)$, then

$$\sup_{|h|<\delta}\int_0^T\int|\rho^\varepsilon(x+h,t)-\rho^\varepsilon(x,t)|dxdt\leq c_0(\log|\log\delta|)^{-1/2}\ H(g). \tag{1.19}$$

On account of Definition 1.1, what we have in mind for g is $Q(f)/(f+1)$. As for ψ, recall

$$\mathcal{L}(f)(x,v,t)=\int\bar{B}(v-v_*)f(x,v,t)\ dv_*,$$

where $\bar{B}(v)=\int B(v,n)\ dn$. This would allow us to obtain the weak regularity of $f\mapsto Q^-(f)/(f+1)$. As for the weak regularity of $Q^+(f)/(f+1)$, we use the weak regularity of $f\mapsto Q^-(f)/(f+1)$, and the entropy production bound of (1.13). After all, if $a=f'f'_*$, and $b=ff_*$, then we use the elementary bound

$$\begin{aligned}a&\leq kb+\frac{a}{b}\ 1\!\!1\left(\frac{a}{b}\geq k\right)\leq kb+(\log k)^{-1}a\log\frac{a}{b}\ 1\!\!1\left(\frac{a}{b}\geq k\right)\\&\leq(\log k-1)^{-1}\ b\left(\frac{a}{b}-1\right)\log\frac{a}{b},\end{aligned}$$

to argue that for an error of order $O\big((\log k)^{-1}\big)$, we can switch from $Q^+(f)/(f+1)$ to $Q^-(f)/(f+1)$.

2 Lorentz Gas

According to Conjecture 1.1, the Boltzmann-Grad limit of the HSM is expected to be governed by Boltzmann equation. In Section 1.3 we gave an overview of the existing results for the Boltzmann equation. A natural question is whether or not some the estimates in Section 1.3 have microscopic counterpart. Indeed this is the case if we add some randomness to the collision mechanism (see [R2] and [RV]). However for the fully deterministic model such as HSM it is an open question to derive Boltzmann equation as in Definition 1.1.

A natural question is whether or not we can bound the total number of collisions. For example, if $\mathcal{N}(T) = \mathcal{N}^\varepsilon(T)$ denotes the total number of collisions that occur in the interval $[0, T]$, a bound of the form

$$\sup_{\varepsilon \in (0,1]} \varepsilon^{d-1} \mathbb{E} \mathcal{N}^\varepsilon(T) < \infty, \tag{2.1}$$

would have the same flavor as $Q^\pm \in L^1$. Perhaps a microscopic counterpart of $Q^\pm \in L^1$ would go as follows: Let us write $\tau_{ij}^1 < \tau_{ij}^2 < \dots$ for the collisions times between i-th and j-th particles. Then we would like to bound

$$\varepsilon^{d-1} \ \mathbb{E} \sum_{i,j} \sum_{k=1}^{\infty} \mathbb{1}\big(\tau_{ij}^k \le T\big) |(v_i - v_j) \cdot n_{ij}|, \tag{2.2}$$

uniformly in ε.

We can use the conservation laws to deduce a weaker bound. To see this observe that if

$$X(t) = \sum_i |x_i(t) - v_i(t)t|^2,$$

then $X(t)$ does not change between collision times, however if τ is a collision time between i-th and j-th particles, then

$$\begin{aligned} X(\tau+) - X(\tau-) &= |x_i - \tau v_i'|^2 + |x_j - \tau v_j'|^2 - |x_i - \tau v_i|^2 - |x_j - \tau v_j|^2 \\ &= -2\varepsilon\tau (v_i' - v_i) \cdot n_{ij} = 2\varepsilon\tau (v_i - v_j) \cdot n_i j, \end{aligned}$$

with all terms on the right-hand side evaluated at $\tau-$ (pre-collisional time). Recall $n_{ij} = (x_i - x_j)/|x_i - x_j|$. Hence $(v_i - v_j) \cdot n_i j \le 0$. From this we deduce

$$\varepsilon^{d-1} \sum_{i,j} \sum_{k=1}^{\infty} \mathbb{1}\big(\tau_{ij}^k \le T\big) \tau_{ij}^k |(v_i - v_j) \cdot n_{ij}| \le \varepsilon^{d-2} X(0). \tag{2.3}$$

Note

$$\iint |x|^2 f^0(x, v)\ dxdv < \infty \quad \implies \quad \sup_{\varepsilon > 0} \mathbb{E} \varepsilon^{d-1} X(0) < \infty,$$

which yields a bound of order $O(\varepsilon^{-1})$ for the right-hand side of (2.3). Perhaps we should mention that mesoscopically, we always have

$$\frac{d}{dt}\iint |x-vt|^2 f(x,v,t)\ dxdv = 0.$$

Microscopically, $X(t)$ is not conserved, though can only increase for an amount of order $O(\varepsilon)$, and this is responsible for our bound (2.3). Needless to say, (2.3) is not good enough for our purposes. A bound on the total number of collisions remains formidable challenge.

We now describe another challenge we encounter as we try to establish Stosszahlensatz. For the validity of Boltzmann equation in Boltzmann-Grad limit, we need to show that recollisions do not occur frequently. We explain this for a variant of HSM that is known as Lorentz gas.

In a Lorenz gas, we have a light particle $(x(t), v(t))$, and immobile particles at locations $x_i,\ i \in I$. The collection $\omega = \omega^\varepsilon = \{x_i :\ i \in I\}$ is random and selected according to a Poisson point process of intensity $\lambda = \varepsilon^{1-d}$. More precisely, if U is a bounded open subset of $\mathbb{R}^d$, and $N(U) = \sharp(\omega \cap U)$, then $\omega \cap U = \{x_1, \dots, x_{N(U)}$ is selected according to the probability measure

$$e^{\varepsilon^{1-d}|U|}\left[1\!\!1(N(U)=0) + \sum_{N=1}^{\infty}(N!)^{-1}\varepsilon^{(1-d)N}1\!\!1(N(U)=N)\ \prod_{i=1}^{N} dx_i\right],$$

where $|U|$ denotes the d-dimensional volume of U. Given a realization of ω, we define of (x,v) for $x \in \Lambda(\omega)$, where

$$\Lambda(\omega) = \big\{x \in \mathbb{R}^d :\ |x - x_i| \ge \varepsilon \ \text{ for } i \in I\big\}.$$

Alternatively, we may replace $\mathbb{R}^d$ with the torus $\mathbb{T}^d$, and assume that $\omega = (x_1, \dots, x_N)$ with $x_1, \dots, x_N$ are selectly intedendent and uniformly from $\mathbb{T}^d$. Again, the relation between ε and N is given by $N = \varepsilon^{1-d}$.

The dynamic of $(x(t), v(t)) = (x(t,\omega^\omega), v(t,\omega^\varepsilon))$ is given by $\dot{x}(t) = v(t),\ \dot{v}(t) = 0$, so long as $x(t)$ is in the interior of $\Lambda(\omega)$. Moreover, when $|x(t) - x_i| = \varepsilon$, for some $i \in I$, then $v(t)$ changes to

$$v(t+) := v(t-) - 2v(t-)\cdot n_i\ n_i,$$

where $n_i = n_i(x) = \varepsilon^{-1}(x - x_i)$.

Theorem 2.1. *(Gallavotti) The process $(x(t,\omega^\omega), v(t,\omega^\varepsilon))$ converges to $\bar{q}(t) = (\bar{x}(t), \bar{v}(t))$, as $\varepsilon \to 0$, where $\bar{q}$ is a Markov process with the infinitesimal generator*

$$\mathcal{A}h(x,v) = v\cdot h_x(x,t) + \int_{\mathbb{S}^{d-1}} (v\cdot n)^-\big(h(x, v - 2(v\cdot n)n) - h(x,v)\big)\ dn.$$

We now provide some heuristics for Theorem 2.1. To simplify the presentation, we consider the periodic version of our model so that the number of particle is $N$and nonrandom.

Let us write $\phi_t(x,v)=\phi_t(x,v;\omega)$ for the flow of $q(t)$. Note that if initially $(x(0),v(0))$ is selected according to $f^0(x,v)\ dxdv$, with f^0 a continuous function, then at later times $(x(t),v(t))$ is distributed according to $f(x,v,t)\ dxdv$, where $f(x,v,t)=f(x,v,t;\omega)$ is given by

$$f(x,v,t)=f^0\big(\phi_t^{-1}(x,v)\big).$$

It is not hard to show

$$\begin{cases} f_t(x,v,t)+v\cdot f_x(x,v,t)=0, & x\in\Lambda(\omega)^o,\\ f(x,v,t)=f\big(x,v-2(v\cdot n_i(x))n_i(x),t\big), & |x-x_i|=\varepsilon. \end{cases} \tag{2.4}$$

Let us write $\chi(x)=\chi(x;\omega)=1\!\!1\big(x\in\Lambda(\omega)\big)$, and

$$\hat f(x,v,t)=\int f(x,v,t;\omega)\chi(x;\omega)\ d\omega.$$

We also write ω^i for $\omega\setminus\{x_i\}$, and $\zeta_i(x,n;\omega)=1\!\!1\big(x=x_i+\varepsilon n\big)$. By divergence theorem,

$$\begin{aligned}\hat f_t+v\cdot\hat f_x&=\int f(v\cdot\nabla\chi)\ d\omega=\varepsilon^{d-1}\sum_i\int\int_{\mathbb{S}^{d-1}}f(x,v,t;\omega)\zeta_i(x,n;\omega)(v\cdot n)\ dn\ d\omega^i\\ &=N\varepsilon^{d-1}\int\int_{\mathbb{S}^{d-1}}f(x,v,t;\omega)\zeta_1(x,n;\omega)(v\cdot n)\ dn\ d\omega^1=Q^+-Q^-,\end{aligned}$$

where

$$\begin{aligned}Q^+&=\int\int_{\mathbb{S}^{d-1}}f(x,v,t;\omega)\zeta_1(x,n;\omega)(v\cdot n)^+\ dn\ d\omega^1,\\ Q^-&=\int\int_{\mathbb{S}^{d-1}}f(x,v,t;\omega)\zeta_1(x,n;\omega)(v\cdot n)^-\ dn\ d\omega^1.\end{aligned}$$

Fix $T>0$, and write Ω_0 for the event of a recollison in $[0,T]$, i.e., the set of ω such that (x,t) collides one of immobile particle twice in $[0,T]$. We also write $\eta=1\!\!1\big(\omega\notin\Omega_0\big)$. Observe that when $\omega\in\Omega_0$, and $v\cdot n_1(x)<0$, we simply have $f(x,v,t;\omega)=f(x,v,t;\omega^1)$. This is because $\phi_t^{-1}(x,v)$ does not encounter x_1 when $\eta=1$. As $\varepsilon\to0$, we have $f(x,v,t;\omega^1)\to\bar f(x,v,t)$, and

$$\lim_{\varepsilon\to0}(\eta Q^-)=\bar f\int_{\mathbb{S}^{d-1}}(v\cdot n)^-\ dn.$$

On the other hand, by the boundary condition in (2.4),

$$Q^+=\int\int_{\mathbb{S}^{d-1}}f(x,v-2(v\cdot n)n,t;\omega)\zeta_1(x,n;\omega)(v\cdot n)^+\ dn\ d\omega^1.$$

We can now can argue as for Q^- to show

$$\lim_{\varepsilon\to 0}(\eta Q^+) = \int_{\mathbb{S}^{d-1}} (v\cdot n)^+ \bar f(x, v-2(v\cdot n)n, t)\ dn,$$

because $\big(v-2(v\cdot n)n\big)\cdot n = -v\cdot n \le 0$. In summary, $\hat f \to \bar f$ in small ε limit, provided that the probability of a recollision is negligible as $\varepsilon \to 0$.

In the case of a Lorentz gas, we can readily show that the times between collisions are distributed as independent exponential random variables, and that the angles between v and n_i's are independent uniformly distributed random variables. A recollison occurs when sum of such angles are almost 2π, and this occurs with negligible probability. It is far more challenging to prove analogous claim in the case of HSM.

3 BBGKY Equations for HSM

Recall that in HSM, we have N particles $\mathbf{z} = \mathbf{z}^N = (z_1, \dots, z_N)$, with $z_i = (x_i, v_i) \in \mathbb{R}^{2d}$. Let us write

$$\hat{\mathbf{z}}^k = (z_{k+1}, \dots, z_N),$$

so that $\mathbf{z} = \mathbf{z}^N = (\mathbf{z}^k, \hat{\mathbf{z}}^k)$. We write

$$\begin{aligned} E_k &= \big\{\mathbf{z}^k = (z_1, \dots, z_k) \in \mathbb{R}^{2kd} :\ |x_i - x_j| \ge \varepsilon \text{ for } \ i \ne j,\ i,j \in \{1, \dots, k\}\big\}, \\ \hat E_k &= \big\{\hat{\mathbf{z}}^k = (z_{k+1}, \dots, z_k) \in \mathbb{R}^{2(N-k)d} :\ |x_i - x_j| \ge \varepsilon \text{ for } \ i \ne j,\ i,j \in \{k+1, \dots, N\}\big\}. \end{aligned}$$

We assume that initially, $\mathbf{z}$ is distributed according to $F^0(\mathbf{z})\ d\mathbf{z}$. At later time, the law of $\mathbf{z}(t)$ is given by $F(\mathbf{z}, t)\ d\mathbf{z}$. We assume that F^0 is symmetric: If we swap x_i with x_j, F^0 does not change. The same holds for F. We may write

$$\partial E_N = \cup_{i\ne j}\partial_{ij} E_N := \cup_{i\ne j}\big(\partial_{ij}^+ E_N \cup \partial_{ij}^- E_N\big),$$

where

$$\partial_{ij}^\pm E_N := \big\{\mathbf{z}^k = (z_1, \dots, z_k) \in E_N :\ |x_i - x_j| = \varepsilon,\ \pm(v_i - v_j)\cdot n_{ij} \ge 0\big\}.$$

As we discussed in Section 2, the function F satisfies a transport equation with boundary conditions:

$$\begin{cases} F_t(\mathbf{z}, t) + \mathbf{v}\cdot F_{\mathbf{x}}(\mathbf{z}, t) = 0, & \mathbf{z} \in E_N^o, \\ F(\mathbf{x}, T^{ij}\mathbf{v}, t) = F(\mathbf{x}, \mathbf{v}, t), & (\mathbf{x}, \mathbf{v}) \in \partial_{ij} E_N, \end{cases} \tag{3.1}$$

where $T^{ij}\mathbf{v}$ is obtained from $\mathbf{v}$ by replacing (v_i, v_j) with (v_i', v_j') as in (1.2). We define

$$F^k(\mathbf{z}^k, t) = \int_{E_N(\mathbf{z}^k)} F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\ d\hat{\mathbf{z}}^k,$$

where

$$E_N(\mathbf{z}^k) = \big\{\hat{\mathbf{z}}^k : \ (\mathbf{z}^k, \hat{\mathbf{z}}^k) \in E_N\big\},$$

for $\mathbf{z}^k \in E_k$. We wish to use (3.1) to derive an equation for F^k. As a preparation, we define

$$\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k) = \prod_{i=1}^{k} \prod_{j=k+1}^{N} \xi^{ij}(x_i, x_j), \qquad \hat{\xi}(\hat{\mathbf{x}}^k) = \prod_{i,j=k+1}^{N} \xi^{ij}(x_i, x_j),$$

where

$$\xi^{ij}(x_i, x_j) = \mathbb{1}\big(|x_i - x_j| \geq \varepsilon\big).$$

With these notations, we may write

$$F^k(\mathbf{z}^k, t) = \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k,$$

for $\mathbf{z}^k \in E_k$. As a result,

$$\begin{aligned}
F_t^k(\mathbf{z}^k, t) + \mathbf{v}^k \cdot F^k_{\mathbf{x}^k}(\mathbf{z}^k, t) =& \int \big(F_t(\mathbf{z}^k, \hat{\mathbf{z}}^k, t) + \mathbf{v}^k \cdot F^k_{\mathbf{x}^k}(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
&+ \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big(\mathbf{v}^k \cdot \xi_{\mathbf{x}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
=& - \int \big(\hat{\mathbf{v}}^k \cdot F_{\hat{\mathbf{x}}^k}(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
&+ \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big(\mathbf{v}^k \cdot \xi_{\mathbf{x}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
=& \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big(\hat{\mathbf{v}}^k \cdot \xi_{\hat{\mathbf{x}}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big)\hat{\xi}(\hat{\mathbf{x}}^k)\big)\ d\hat{\mathbf{z}}^k \\
&+ \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big(\hat{\mathbf{v}}^k \cdot \hat{\xi}_{\hat{\mathbf{x}}^k}(\hat{\mathbf{x}}^k)\big)\ d\hat{\mathbf{z}}^k \\
&+ \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\big(\mathbf{v}^k \cdot \xi_{\mathbf{x}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big)\hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
=& \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\ \big(\mathbf{v}^k \cdot \xi_{\mathbf{x}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k) + \hat{\mathbf{v}}^k \cdot \xi_{\hat{\mathbf{x}}^k}(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big)\ \hat{\xi}(\hat{\mathbf{x}}^k)\ d\hat{\mathbf{z}}^k \\
&+ \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big(\hat{\mathbf{v}}^k \cdot \hat{\xi}_{\hat{\mathbf{x}}^k}(\hat{\mathbf{x}}^k)\big)\ d\hat{\mathbf{z}}^k \\
=:& X_1 + X_2,
\end{aligned}$$

where we used (3.1) for the second equality, and integrated by parts for the third equality. We claim that $X_2 = 0$. To see this, for distinct $i, j \in \{k+1, \dots, N\} =: \hat{I}_k$, we define

$$X_2^{ij} := \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\big(v_i \cdot \xi^{ij}_{x_i}(x_i, x_j) + v_j \cdot \xi^{ij}_{x_j}(x_i, x_j)\big)\ dz_i dz_j.$$

For $X_2 = 0$, we simply show that $X_2^{ij} = 0$ for every distinct pair of $i, j \in \hat{I}_k$. Indeed,

$$X_2^{ij} = \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k) \left((v_i - v_j) \cdot n_{ij} \right) \ \sigma_{ij}(dx_i, dx_j) \ dv_i dv_j, \tag{3.2}$$

where σ_{ij} is the surface measure on the set $\{(x_i, x_j) : \ |x_i - x_j| = \varepsilon\}$. We now perform a change of variables $(v_i, v_j) \to (v_i', v_j')$ in the integral on the right-hand side of (3.2). This change of variable is of Jacobian 1, and does not change the $F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)$ term because of the boundary conditions in (3.1). However, it changes $(v_i - v_j) \cdot n_{ij}$ to $(v_i' - v_j') \cdot n_{ij} = -(v_i - v_j) \cdot n_{ij}$, which results in the equality $X_2^{ij} = -X_2^{ij}$. This confirms our claim $X_2^{ij} = 0$.

We now turn our attention to X_1. For any $(i, j) \in \{1, \dots, k\} \times \{k + 1, \dots, N\}$, we have

$$\begin{aligned} X_1^{ij} &:= \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\left(v_i \cdot \xi_{x_i}^{ij}(x_i, x_j) + v_j \cdot \xi_{x_j}^{ij}(x_i, x_j)\right) \ dz_j \\ &= \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t)\xi(\mathbf{x}^k, \hat{\mathbf{x}}^k) \left((v_i - v_j) \cdot n_{ij} \right) \ \sigma_j^i(x_i, dx_j) \ dv_j, \end{aligned}$$

where $\sigma_j^i(x_i, dx_j)$ is the surface measure on the set $\{x_j : \ |x_i - x_j| = \varepsilon\}$. From this we deduce

$$X_1 = \sum_{i=1}^{k} \sum_{j=k+1}^{N} \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t) \left((v_i - v_j) \cdot n_{ij} \right) \xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\hat{\xi}(\hat{\mathbf{x}}^k) \ \sigma_j^i(x_i, dx_j) \ dv_j \prod_{r \in \hat{I}^k \setminus \{j\}} dz_r.$$

We then use the symmetry of F to assert that X_1 equals to

$$(N - k) \sum_{i=1}^{k} \int F(\mathbf{z}^k, \hat{\mathbf{z}}^k, t) \left((v_i - v_{k+1}) \cdot n_{i,k+1} \right) \xi(\mathbf{x}^k, \hat{\mathbf{x}}^k)\hat{\xi}(\hat{\mathbf{x}}^k) \ \sigma_{k+1}^i(x_i, dx_{k+1}) \ dv_{k+1} \ d\hat{\mathbf{z}}^{k+1}$$

We may rewrite this as

$$(N-k)\varepsilon^{d-1} \sum_{i=1}^{k} \int \int_{\mathbb{S}^{d-1}} F^{k+1}(\mathbf{z}^k, x_i - \varepsilon n, v_{k+1}, t) \left((v_i - v_{k+1}) \cdot n \right) \ dn dv_{k+1} =: \lambda_k \left(C_k^{k+1} F^{k+1} \right)(\mathbf{z}^k, t),$$

where $\lambda_k = \lambda^\varepsilon = (N - k)\varepsilon^{d-1}$. Note that an assumption of the form $N = \lambda\varepsilon^{1-d}$ leads to $\lambda_k^\varepsilon \to \lambda$ as $\varepsilon \to 0$. In summary, we have derived the BBGKY equation

$$\begin{cases} F_t^k(\mathbf{z}^k, t) + \mathbf{v}^k \cdot F_{\mathbf{x}^k}^k(\mathbf{z}^k, t) = \lambda_k \left(C_k^{k+1} F^{k+1} \right)(\mathbf{z}^k, t), & \mathbf{z}^k \in E_k^o, \\ F^k(\mathbf{x}^k, T^{ij}\mathbf{v}^k) = F^k(\mathbf{x}^k, \mathbf{v}^k, t), & \mathbf{z}^k \in \partial_{ij} E_k. \end{cases} \tag{3.3}$$

As in Section 2, we write $C_k^{k+1} = Q_k^+ - Q_k^-$, where

$$\begin{aligned} Q_k^- h(\mathbf{z}^k) &= \sum_{i=1}^{k} \int \int_{\mathbb{S}^{d-1}} h(\mathbf{z}^k, x_i - \varepsilon n, v_{k+1}, t) \left((v_i - v_{k+1}) \cdot n \right)^- \ dn dv_{k+1}, \\ Q_k^+ h(\mathbf{z}^k) &= \sum_{i=1}^{k} \int \int_{\mathbb{S}^{d-1}} h(T_n^i \mathbf{z}^k, x_i - \varepsilon n, v_{k+1}', t) \left((v_i - v_{k+1}) \cdot n \right)^- \ dn dv_{k+1}, \end{aligned}$$

where $v'_{k+1} = v_{k+1} + (v_i - v_{k+1}) \cdot n\ n$, and $T_n^i \mathbf{z}^k$ is obtained from $\mathbf{z}^k$ by replacing v_i with $v'_i = v_i - (v_i - v_{k+1}) \cdot n\ n$. Let us write ϕ_t^k for the flow of $\mathbf{z}_k$, (ignoring the interaction between $\mathbf{z}^k$ and $\hat{\mathbf{z}}^k$), and define $S_t^k h := h \circ \phi_t^k$. We can then apply Duhamel's formula to (3.3) to assert

$$F_t^k(\mathbf{z}^k, t) = \left(S_t^k F_0^k\right)(\mathbf{z}^k) + \lambda_k \int_0^t \left(S_{t-t_1}^k C_k^{k+1} F^{k+1}\right)(\mathbf{z}^k, t_1)\ dt_1, \tag{3.4}$$

where $F_0^k(\mathbf{z}^k) = F^k(\mathbf{z}^k, 0)$. We may apply Duhamel's formula to (3.4), and after an induction we learn that $F^k(\mathbf{z}^k, t)$ equals to

$$\left(S_t^k F_0^k\right)(\mathbf{z}^k) + \sum_{m=1}^{N-k} \lambda_k^m \int_{\Delta_m(t)} \left(S_{t-t_1}^k C_k^{k+1} S_{t_1-t_2}^{k+1} \dots C_{k+m-1}^{k+m} S_{t_m}^{k+m} F_0^{k+m}\right)(\mathbf{z}^k) \prod_{i=1}^m dt_i, \tag{3.5}$$

where $\lambda_k^m = \lambda_k \dots \lambda_{k+m-1}$, and

$$\Delta_m(t) = \left\{(t_1, \dots, t_m) :\ t \geq t_1 \geq \dots t_m \geq 0\right\}.$$

The formula (3.5) suggests a strategy for tackling Conjecture 1.1. Note that if we can show

$$\lim_{\varepsilon \to \infty} F^1(z_1, t) = \lambda^{-1} f(z_1, t), \qquad \lim_{\varepsilon \to \infty} F^2(z_1, z_2, t) = \lambda^{-2} f(z_1, t) f_2(z_2), \tag{3.6}$$

then by standard arguments we can readily establish (1.3). More generally, we may try to show

$$\lim_{\varepsilon \to \infty} F^k(z^k, t) = \lambda^{-k} \prod_{i=1}^k f(z_i, t). \tag{3.7}$$

On account of (3.5), we may achieve (3.7) in three steps:

(i) We show that in the small ε limit, the operator S_t^k converges to $\bar{S}_t^k$, where

$$\left(\bar{S}_t^k h\right)(\mathbf{x}^k, \mathbf{v}^k) = h(\mathbf{x}^k - t\mathbf{v}^k, \mathbf{v}^k). \tag{3.8}$$

(ii) We show that in the small ε limit, the operator $Q_k^\pm$ converges to $\bar{Q}_k^\pm$, where

$$\left(\bar{Q}_k^- h\right)(\mathbf{x}^k, \mathbf{v}^k) = \sum_{i=1}^k \int \int_{\mathbb{S}^{d-1}} \left((v_i - v_{k+1}) \cdot n\right)^- h(\mathbf{z}^k, x_i, v_{k+1}, t)\ dn d_{v_{k+1}}, \tag{3.9}$$

and $\bar{Q}_k^+$ is defined as in (3.9), except that we replace (v_i, v_{k+1}) in the argument of h with (v'_i, v'_{k+1}).

(iii) We show that the series is absolutely convergent as $N \to \infty$.

It turns out the crucial step is **(iii)**, which allow us to replace the large sum in (3.5) with a fixed finite sum for a small error. Once this is achieved, it is not hard to verify **(i)** and **(ii)** in this finite sum because each term in the summand involves finitely many particles. That is, we only send $\varepsilon \to 0$ in **(i)** and **(ii)**, while the number of particles is fixed. Indeed if there are $\ell = k + m$ many particles, then the probability of a collision in an interval $[0, T]$ goes to 0 as $\varepsilon \to 0$. We are now ready to sketch the proof of Theorems 1.1.

Proof of Theorem 1.1 On account of our discussion above, we only need to verify absolute convergence of the series in (3.5). Our initial density is given by (1.7) with f^0 that satisfies

$$f^0(z_1) \le AM_\theta(v_1) := A(2\pi\theta)^{-d/2} e^{-\frac{|v_1|^2}{2\theta}}. \tag{3.10}$$

From this, it is not hard to deduce that there exists a constant A such that

$$F_0^\ell(\mathbf{z}^k) := F^\ell(\mathbf{z}^k, 0) \le A^\ell \prod_{i=1}^{\ell} M_\theta(v_i) =: A^\ell M_\theta^\ell(\mathbf{v}^\ell). \tag{3.11}$$

Clearly the operator S_t does not alter the right-hand side by the conservation of energy:

$$(S_t^\ell F_0^\ell)(\mathbf{z}^k) \le A^\ell M_\theta^\ell(\mathbf{v}^\ell). \tag{3.12}$$

Let us first replace $\big((v_i - v_*)\cdot n\big)^-$ in the definition of $Q_k^\pm$ with a bounded function $B(v_i - v_*, n)$. We can then assert

$$\big(Q_{\ell-1}^\pm S_t^\ell F_0^\ell\big)(\mathbf{z}^k) \le c_0 B_0 (\ell - 1) A^\ell \prod_{i=1}^{\ell-1} M_\theta(v_i),$$

where B_0 is an upper bound for B, and c_0 is the total measure of $\mathbb{S}^{d-1}$. From this and (3.5) we arrive at a bound of the form

$$\begin{aligned} F^k(\mathbf{z}^k, t) \le& A^k M_\theta^k(\mathbf{v}^k) \left[1 + \sum_{m=1}^{N-k} \lambda^m A^m (c_0 B_0)^m \big(k(k+1)\dots(k+m-1)\big)\frac{t^m}{m!}\right] \\ \le& A^k M_\theta^k(\mathbf{v}^k) \left[1 + \sum_{m=1}^{N-k} (2\lambda A c_0 B_0 t)^m\right]. \end{aligned} \tag{3.13}$$

From this it is clear that the expression in the brackets is uniformly bounded if $2\lambda A c_0 B_0 t < 1$.

For HSM, B is not bounded. To deal with it, we borrow from our Maxwellian to bound this. To see this, observe that for and $\alpha > 0$,

$$\sum_{i=1}^{\ell} |v_i| e^{-\alpha|\mathbf{v}^\ell|^2} \le \alpha^{-1/2} \max_{\mathbf{v}^\ell} \left[\sum_{i=1}^{\ell} |v_i| e^{-|\mathbf{v}^\ell|^2}\right] \le \alpha^{-1/2}\ell^{1/2} \max_{\mathbf{v}^\ell} \left[|\mathbf{v}^\ell| e^{-|\mathbf{v}^\ell|^2}\right] = c_1 \alpha^{-1/2} \ell^{1/2},$$

for $c_1 = 2^{-1/2}e^{-1/2}$. From this we deduce that for $\alpha, \beta > 0$,

$$\begin{aligned}\sum_{i=1}^{\ell} |v_i - v_{\ell+1}| \; e^{-\alpha|\mathbf{v}^\ell|^2 - \beta v_{\ell+1}^2} &\le \sum_{i=1}^{\ell} (|v_i| + |v_{\ell+1}|) \; e^{-\alpha|\mathbf{v}^\ell|^2 - \beta v_{\ell+1}^2} \\ &\le c_1\big[\alpha^{-1/2}\ell^{1/2} + \beta^{-1/2}\ell\big].\end{aligned}$$

As a result,

$$\prod_{\ell=k}^{k+m-1} \sum_{i=1}^{\ell} |v_i - v_{\ell+1}| \; \exp\left[-\sum_{\ell=k}^{k+m-1} \left(\alpha|\mathbf{v}^\ell|^2 + \beta v_{\ell+1}^2\right)\right] \le c_1^{m-1} \prod_{\ell=k}^{k+m-1} \left[\alpha^{-1/2}\ell^{1/2} + \beta^{-1/2}\ell\right]$$

This in turn implies

$$\prod_{\ell=k}^{k+m-1} \sum_{i=1}^{\ell} |v_i - v_{\ell+1}| \; \exp\left[-\big((m-1)\alpha + \beta\big) \; |\mathbf{v}^{k+m}|^2\right] \le c_1^{m-1} \prod_{\ell=k}^{k+m-1} \left[\alpha^{-1/2}\ell^{1/2} + \beta^{-1/2}\ell\right]$$

If we choose $\alpha = \beta/(m-1)$, we obtain

$$\begin{aligned}\prod_{\ell=k}^{k+m-1} \sum_{i=1}^{\ell} |v_i - v_{\ell+1}| \; \exp\left[-2\beta|\mathbf{v}^{k+m}|^2\right] &\le \big(c_1\beta^{-1/2}\big)^{m-1} \prod_{\ell=k}^{k+m-1} \left[(m-1)^{1/2}\ell^{1/2} + \ell\right] \\ &\le \big(2c_1\beta^{-1/2}(k+m-1)\big)^{m-1}.\end{aligned}$$

In summary,

$$\prod_{\ell=k}^{k+m-1} \sum_{i=1}^{\ell} |v_i - v_{\ell+1}| \le \big(2c_1\beta^{-1/2}(k+m-1)\big)^{m-1} \exp\left[2\beta|\mathbf{v}^{k+m}|^2\right]. \tag{3.14}$$

We now choose $\beta \in \big(0, (4\theta)^{-1}\big)$ in (3.14) to assert that the expression

$$\big(S_{t-t_1}^k C_k^{k+1} S_{t_1-t_2}^{k+1} \dots C_{k+m-1}^{k+m} S_{t_m}^{k+m} F_0^{k+m}\big)(\mathbf{z}^k),$$

is bounded above by

$$\begin{aligned}A^k M_\theta^k(\mathbf{v}^k) e^{2\beta|\mathbf{v}^k|^2} \big(2c_1\beta^{-1/2}(k+m-1)\big)^{m-1} (c_0 A)^m \int \prod_{j=k+1}^{k+m} \left[M_\theta(v_j) e^{2\beta|v_j|^2} \; dv_j\right] \\ \le A^k M_\theta^k(\mathbf{v}^k) e^{2\beta|\mathbf{v}^k|^2} \big(2c_1\beta^{-1/2}(k+m-1)\big)^{m-1} (c_0 A)^m (1-4\theta\beta)^{-m/2} \\ =: A^k M_\theta^k(\mathbf{v}^k) e^{2\beta|\mathbf{v}^k|^2} (k+m-1)^{m-1} c_2^m.\end{aligned}$$

This and (3.5) allow us to assert

$$F^k(\mathbf{z}^k,t) \le A^k M_\theta^k(\mathbf{v}^k) + A^k M_\theta^k(\mathbf{v}^k) e^{2\beta|\mathbf{v}^k|^2} \sum_{m=1}^{N-k} \left[\lambda^m c_2^m (k+m-1)^{m-1} \frac{t^m}{m!} \right].$$

We then use Stirling's formula to assert that there exists c_3 such that

$$F^k(\mathbf{z}^k,t) \le A^k M_\theta^k(\mathbf{v}^k) + A^k M_\theta^k(\mathbf{v}^k) e^{2\beta|\mathbf{v}^k|^2} \sum_{m=1}^{N-k} (c_3 t)^m.$$

From this we conclude that if $c_3 t < 1$, and $\bar\theta = \left(\theta^{-1} - 4\beta\right)^{-1}$, then we can find a constant $\bar A$ such that

$$F^k(\mathbf{z}^k,t) \le \bar A^k M_{\bar\theta}^k(\mathbf{v}^k),$$

for every $k \in \{1,\dots,N\}$. □

4 Cumulant Bounds

So far we have assumed that total number of particles is fixed in our HSM. To allow more flexibility, we choose a state space

$$\mathcal{E} = \left\{\omega \subset \mathbb{R}^{2d} : \ \mathcal{N}(\omega) := \sharp\omega < \infty\right\}.$$

To have a probability measure $\mathbb{P}$ on $\mathcal{E}$, we start with a family of measurable symmetric functions

$$W_m : \mathbb{R}^{2dm} \to [0,\infty), \quad m \in \mathbb{N},$$

and set

$$\mathbb{P}\big(\mathcal{N}(\omega) = m, \ \omega = \{z_1,\dots,z_m\} \in A\big) = \frac{1}{m!} \int_A W_m(z_1,\dots,z_m) \ dz_1 \dots dz_m,$$

for $m \in \mathbb{N}$ and $A \subseteq \mathbb{R}^{2dm}$. Additionally, we need a constant $p_0 \in [0,1]$ to represents the probability of $\mathcal{N}(\omega) = 0$. Note that if

$$p_m := \mathbb{P}(\mathcal{N} = m) = \frac{1}{m!} \int_{\mathbb{R}^{2dm}} W_m(z_1,\dots,z_m) \ dz_1 \dots dz_m,$$

for $m \in \mathbb{N}$, then we must have

$$\sum_{m=0}^{\infty} p_m = 1.$$

The probability measure $\mathbb{P}$ is an example of (finite) point process, and $(W_m:\ m\in\mathbb{N}_*)$ are known as *Janossy functions*. The corresponding correlation functions are defined by

$$\rho_k(\mathbf{z}^k)=\rho(z_1,\dots,z_k):=W_k(\mathbf{z}^k)+\sum_{\ell=1}^{\infty}\frac{1}{\ell!}\int_{\mathbb{R}^{2(k+\ell)d}}W_{k+\ell}(\mathbf{z}^{k+\ell})\ \prod_{i=1}^{\ell}dz_{k+i}. \tag{4.1}$$

Note

$$\mathbb{E}\sum\ \big\{h(z_1,\dots,z_k):\ z_1\neq\dots\neq z_k,\ \{z_1,\dots,z_k\}\subseteq\omega\big\}=\int\rho_k(\mathbf{z}^k)\ h(\mathbf{z}^k)\ d\mathbf{z}^k.$$

Moreover,

$$\int\rho_k(\mathbf{z}^k)\ d\mathbf{z}^k=\mathbb{E}\big[\mathcal{N}(\mathcal{N}-1)\dots(\mathcal{N}-k+1)\ \mathbb{1}(\mathcal{N}\geq k)\big].$$

For our HSM, we may start with an initial probability measure $\mathbb{P}_0=\mathbb{P}_0^\varepsilon$ such that

$$\lim_{\varepsilon\to0}\varepsilon^{d-1}\mathbb{E}^\varepsilon\ \mathcal{N}=\lambda\in(0,\infty), \tag{4.2}$$

where $\mathbb{E}^\varepsilon$ denoted the expected value with respect to $\mathbb{P}_0^\varepsilon$.

Given $f^0(z)$, we define $\mathbb{P}_0=\mathbb{P}_0^\varepsilon$ to be the point process associated with Janossy functions

$$W_m^0(\mathbf{z}^m)=Z_\varepsilon^{-1}\varepsilon^{(1-d)m}\ \chi_m(\mathbf{z}^m)\prod_{i=1}^{m}f^0(z_i),$$

where

$$\chi_m(\mathbf{z}^m)=\mathbb{1}\big(|x_i-x_j|\geq\varepsilon\ \text{ for }\ i\neq j,\ i,j\in[m]\big),$$

with $[m]:=\{1,\dots,m\}$, and

$$Z_\varepsilon=1+\sum_{m=1}^{\infty}\frac{\varepsilon^{(1-d)m}}{m!}\int\chi_m(\mathbf{z}^m)\prod_{i=1}^{m}f^0(z_i)\ d\mathbf{z}^m.$$

One can show that (4.2) holds for $\lambda=\int f^0\ dz$.

The configuration $\omega=\omega(0)$ evolves with time according to the HSM dynamics. The configuration $\omega(t)=\{z_1(t),\dots,z_N(t)\}$ is distributed according to the probability measure $\$\mathbb{P}_t^\varepsilon$, which is a point process associated with Janossy functions

$$W_m(\mathbf{z}^m,t)=W_m\big(\phi_t^{-1}(\mathbf{z}^m)\big). \tag{4.3}$$

In the case of HSM, the analog of F^k of Section 3 is given by

$$F^{\varepsilon,k}(\mathbf{z}^k,t)=F^k(\mathbf{z}^k,t)=\varepsilon^{(d-1)k}\rho_k^\varepsilon(\mathbf{z}^k,t),$$

where $\rho_k^\varepsilon(\mathbf{z}^k,t)$ is defined as in (4.1) for W_k as in (4.3).

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