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Propagation of Chaos for Kac-like Particle Models

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Abstract

This thesis concerns various aspects of the Kac model. The Kac model is a Markov jump process for a particle system where the total kinetic energy of the system is conserved. This particle model is connected to a limiting equation, describing the evolution of a one-particle density, when the numbers of particles tends to infinity. To rigourously derive the limiting equation, Kac proved that propagation of chaos holds for his model. Vaguely speaking, here chaos or chaotic means that the two-particle density can be written as a product of two one-particle densities when the numbers of particles tends to infinity. Propagation of chaos means that this property is propagated in time. The thesis contains three papers.

The thermosttated Kac model is particle model where the jumps are modeled as in the Kac model. In additions to the jumps, the particles are accelerated between the jumps under the presence of a uniform force with a thermostat, acting equally on all particles. The thermostat ensures that no extra energy is supplied into the system by the force. In paper I we show that propagation of chaos holds for the thermosttated Kac model.

In paper II we study a modified Kac model where the expression for the kinetic energy of a particle is replaced by an arbitrary energy function. This includes a one-dimensional Kac model for relativistic particles. We show that uniform distribution on the manifold defined by the conservation of total energy is chaotic. We also show that propagation of chaos holds for these modified Kac models.

The BGK equation is an approximation to the Boltzmann equation by a relaxation term. In paper III we study a particle model involving jumps and exchanges between particles. We show that this particle model is connected to the one-dimensional spatially homogeneous BGK equation when the numbers of particles tends to infinity.

Keywords: Master equations, chaotic densities, kinetic equations, propagation of chaos, Kac model, thermostatted master equation, Boltzmann equation, BGK equation, quenched process, uniform distribution, spectral gap, approximation process

Preface

This thesis consists of the following papers.

- ▹ Eric Carlen, Dawan Mustafa and Bernt Wennberg,
  "*Propagation of Chaos for the Thermostatted Kac Master Equation*",
  in *J Stat Phys* **158** (2015), no. 6, 1341–1378.

- ▹ Dawan Mustafa and Bernt Wennberg,
  "*Chaotic distributions for relativistic particles*",
  accepted for publication subject to minor revisions.

- ▹ Dawan Mustafa and Bernt Wennberg,
  "*A many particle model for the BGK equation*",
  preprint.

Acknowledgements

I appreciate the value of learning new things and always try to push myself a little bit more. Looking back in time, I think this is the reason why I wanted to do a Ph.D. in mathematics

During this time, the struggle with mathematical problems have been a recurring theme on daily basis. In order to take a small step forward I first had to face many setbacks. But each day has been an adventure and enormously rewarding thanks to the support of great friends and fantastic colleagues.

First and foremost, I would like to express my deepest gratitude to my advisor, Bernt Wennberg. Your attitude towards mathematics and life in general is a great source of inspiration. Thank you, Bernt, for your unwavering support and patience. I am incredibly lucky to have had you as my advisor and mentor

Peter, we have now shared office for more than five years. It has been a pleasure. With you by my side, I have found the courage to keep trying during difficult moments. Your friendship is substantial to me.

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Dawan Mustafa
Göteborg, November 2015

Contents

Part I

INTRODUCTION

Introduction

1. Overview

In many situations regarding a mathematical model of the real world, one needs to take into account the large number of particles (elements) the system is composed of. In a mechanical system, a gas is composed of more than $N \sim 10^{19}$ particles (molecules) in a volume of 1 cm^3, galaxies are made of hundreds billions of stars. From the point of view in biology, a population may consist of millions of individuals. Tracking the motion of each particle in a gas is a very difficult task if not impossible. To begin with, one needs to specify initial information of positions and velocities of all the particles. This is enormously difficult due to the large number of particles the gas is composed of. Even if initial data is specified, one has to use a computer to solve $3N + 3N$ equations to determine the evolution of the positions and velocities of the particles. There are no powerful enough computers to handle this in a reasonable time amount.

In statistical mechanics powerful methods and tools have been developed during the years to replace the complicated description of a system consisting of a large number of particles in terms of averages. The aim is to explain observable and measurable quantities on the basis of the behaviour of the particles (atoms) in the system. These averages are in some cases described by time evolution equations called kinetic equations. In the kinetic theory of dilute gases, one such famous equation is the Boltzmann equation, and for the motion of galaxies , the Vlasov equation.

The original derivation of the Boltzmann equation is based of on the physical laws of the pairwise interaction between particles in the gas. Although, extensive research has been done, up until today, a satisfactory mathematical derivation of the Boltzmann equation, valid over a macroscopic time interval, is an important open mathematical problem.

In 1956, Mark Kac published a paper, foundations of kinetic theory, [**22**], in which a derivation of the Boltzmann equation is proposed by probabilistic methods. This thesis is devoted to the derivation of some kinetic equations based on the probabilistic methods introduced by Kac.

2. Kinetic theory

At a macroscopic scale, a gas is described by quantities, such as macroscopic density, bulk velocity, pressure, temperature, heat flow, and mean velocity. The equations of motions are given by the Navier-Stokes and Euler equations. At a microscopic scale, the gas is described in terms of the interactions of the molecules the gas is composed of, the equations of motions are given by Newton's equations. Kinetic theory is concerned with a description of the gas between these two scales, a mesoscopic scale. The main idea is to use a statistical description of the gas in terms of a distribution function f which in mathematical literature usually is interpreted as a *one particle distribution*, giving the probability of finding one particle in a specified volume of phase space. More precisely, the goal is to obtain an evolution equation of the non-negative distribution function $f(\boldsymbol{x},\boldsymbol{v},t)$ defined on $\Omega\times\mathbb{R}^3\times\mathbb{R}^+$, $\Omega\subset\mathbb{R}^3$. The variables $\boldsymbol{x}$, $\boldsymbol{v}$, t represent respectively, position, velocity and time. The function f can also be interpreted as the number density, i.e., the expected number of particles that can be found in a given volume of phase space: Assume that the gas consists of N particles, which in the sequel we assume that all are identical particles, i.e, all particles have the same mass. Then at time t,

$$\int_A\int_B f(\boldsymbol{x},\boldsymbol{v},t)\,d\boldsymbol{x}\,d\boldsymbol{v},\qquad A\times B\subset\mathbb{R}^3\times\mathbb{R}^3$$

gives the expected number of particles having positions and velocities $(\boldsymbol{x},\boldsymbol{v})\in A\times B$. The number of particles N is assumed to be very large. The evolution equation for $f(\boldsymbol{x},\boldsymbol{v},t)$ together with boundary conditions is enough to a give sufficient description of the gas. The reason is that the gas is made of such a large number of particles that it can be regarded as a continuum and f is a good approximation to the true density on a macroscopic scale. The macroscopic quantities are computed in terms of the moments of f.

To derive the evolution equation of f, we consider first the case where there no collisions and external forces. Then, the particles move along a straight line, i.e., a particle having position and velocity $(\boldsymbol{x},\boldsymbol{v})$ at time t_0 moves to $(\boldsymbol{x}+(t-t_0)\boldsymbol{v},\boldsymbol{v})$ at time t. The distribution function f remains constant along this line, i.e.,

$$f(\boldsymbol{x},\boldsymbol{v},t)=f(\boldsymbol{x}-(t-t_0)\boldsymbol{v},\boldsymbol{v},t_0).$$

The time evolution equation of f is

$$\frac{\partial}{\partial t}f(\boldsymbol{x},\boldsymbol{v},t)+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}f(\boldsymbol{x},\boldsymbol{v},t)=0. \tag{2.1}$$

This evolution is known as the equation of free transport. If an external force $\boldsymbol{G}(\boldsymbol{x})$ acts on the particles, then evolution equation for the distribution reads

$$\frac{\partial}{\partial t}f(\boldsymbol{x},\boldsymbol{v},t)+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}f(\boldsymbol{x},\boldsymbol{v},t)+\boldsymbol{G}(\boldsymbol{x})\cdot\nabla_{\boldsymbol{v}}f(\boldsymbol{x},\boldsymbol{v},t)=0.$$

This is the case of the Vlasov equation and here it is assumed that $\boldsymbol{G}$ is a divergence free force field.

Taking into account the effect of collisions between the particles correspond to replacing the right hand side of equation (2.1) by an operator $Q(f,f)$, called the collision integral, describing the change of the distribution under the influence of binary collisions between particles. The collision operator will be described below. The evolution equation for f becomes

$$\frac{\partial}{\partial t}f(\boldsymbol{x},\boldsymbol{v},t)+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}f(\boldsymbol{x},\boldsymbol{v},t)=Q(f,f)(\boldsymbol{x},\boldsymbol{v},t). \tag{2.2}$$

This equation is known as the Boltzmann equation. It was derived by L. Boltzmann in 1872. In fact, the weak form of the Boltzmann equation was derived by J.C. Maxwell in 1967. The left hand side of equation (2.2) corresponds to the free flow of the particles, and the right hand side counts the influence of the binary collisions between the particles. The equation taking into account only the effect of binary collisions but no transport is known as the *spatially homogeneous* Boltzmann equation, and is given by

$$\frac{\partial}{\partial t}f(\boldsymbol{v},t)=Q(f,f)(\boldsymbol{v},t). \tag{2.3}$$

For a thorough discussion on the Boltzmann, the interested reader may consult the classical references [**11**] and [**13**]. For rather recent thorough survey on the Boltzmann equation, see [**32**].

In the remaining part of this introduction, only the spatially homogeneous case is considered. The collision integral has the following structure

$$Q(f,f)(\boldsymbol{v},t)=\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left(f'f'_*-ff_*\right)B(|\boldsymbol{v}-\boldsymbol{v}_*|,\boldsymbol{\sigma})\,d\boldsymbol{\sigma}\,d\boldsymbol{v}_*, \tag{2.4}$$

where the notations f, f_*, f' and f'_* specify respectively, $f(\boldsymbol{v},t)$, $f(\boldsymbol{v}_*,t)$, $f(\boldsymbol{v}',t)$ and $f(\boldsymbol{v}'_*,t)$. The pair of velocities $(\boldsymbol{v},\boldsymbol{v}_*)$ represent the velocities of two particles after a collision, and the pair $(\boldsymbol{v}',\boldsymbol{v}'_*)$ the velocities of these two particles before the collision. The collisions are assumed to be elastic, i.e., collisions preserve momentum and energy:

$$\boldsymbol{v}+\boldsymbol{v}_* = \boldsymbol{v}'+\boldsymbol{v}'_* \qquad \text{and} \qquad |\boldsymbol{v}|^2+|\boldsymbol{v}_*|^2 = |\boldsymbol{v}'|^2+|\boldsymbol{v}'_*|^2.$$

The pair $(\boldsymbol{v},\boldsymbol{v}_*)$ defines a sphere with center at $\frac{\boldsymbol{v}+\boldsymbol{v}_*}{2}$ and diameter $|\boldsymbol{v}-\boldsymbol{v}_*|$, with the pair $(\boldsymbol{v}',\boldsymbol{v}'_*)$ being antipodes on that sphere. A parametrization by a unit vector $\boldsymbol{\sigma}\in\mathbb{S}^2$ leads to

$$\boldsymbol{v}' = \frac{\boldsymbol{v}+\boldsymbol{v}_*}{2}+\frac{|\boldsymbol{v}-\boldsymbol{v}_*|}{2}\boldsymbol{\sigma} \qquad \text{and} \qquad \boldsymbol{v}'_* = \frac{\boldsymbol{v}+\boldsymbol{v}_*}{2}-\frac{|\boldsymbol{v}-\boldsymbol{v}_*|}{2}\boldsymbol{\sigma}.$$

In short, the collision integral (2.4) describes the loss of particles with velocity $\boldsymbol{v}$ due to collisions with particles having velocity $\boldsymbol{v}_*$, and the gain of particles with velocity $\boldsymbol{v}$ due to collisions of particles having velocities $\boldsymbol{v}'$ and $\boldsymbol{v}'_*$. The fact the collision integral involves products of the distribution f is a consequence of Boltzmann's *stosszahlansatz* assumption, the assumption that two particles before a collision are uncorrelated. The rate at which pairs of velocities in a given range collide depends on the kind of interaction between the particles in the gas and this is described by the function $B(|\boldsymbol{v}-\boldsymbol{v}_*|,\boldsymbol{\sigma})$, called the collision kernel. In some cases B can be computed explicitly. In the case of interaction between hard sphere particles

$$B(|\boldsymbol{v}-\boldsymbol{v}_*|,\boldsymbol{\sigma}) = b_0|\boldsymbol{v}-\boldsymbol{v}_*|,$$

where b_0 is a parameter related to the surface area of a hard sphere.

If the interaction is instead given by an inverse power law, then

$$B(|\boldsymbol{v}-\boldsymbol{v}_*|,\boldsymbol{\sigma}) = |\boldsymbol{v}-\boldsymbol{v}_*|^r\, b(\cos\theta),$$

where the scattering angle θ is the angle between $\boldsymbol{v}-\boldsymbol{v}_*$ and $\boldsymbol{v}'-\boldsymbol{v}'_*$, that is

$$\cos\theta = \left\langle \frac{\boldsymbol{v}-\boldsymbol{v}_*}{|\boldsymbol{v}-\boldsymbol{v}_*|},\boldsymbol{\sigma}\right\rangle,$$

with $r=\frac{s-5}{s-1}$ and $s>2$. The function b is implicitly defined and has a non-integrable singularity as $\theta\to 0$:

$$\sin\theta\ b(\cos\theta)\sim\theta^{-1-\nu},$$

where $\nu=\frac{2}{s-1}$. It is common to impose a *cut-off* condition which means that $\sin\theta\ b(\cos\theta)$ is integrable near $\theta=0$. The interaction is said to be hard potential if $s > 5$, and soft potential if $s > 5$. The case $s = 5$ is known as a maxwellian interaction. The maxwellian interaction is independent of the relative velocities. In this case

$$B(|v - v_*|, \boldsymbol{\sigma}) = b(\cos\theta),$$

and under the assumption that, $\sin\theta \ b(\cos\theta)$ is integrable, the interaction is called cut-off maxwellian.

The conservation laws of the spatially homogeneous Boltzmann equation are determined by the properties of the collision integral. To see which quantities are conserved, let $\phi(\boldsymbol{v})$ be a function of $\boldsymbol{v}$ such that the indicated integrals exist. By repeated change of variables, the collision integral satisfies

$$\begin{aligned}(2.5)\qquad &\int_{\mathbb{R}^3} Q(f,f)(\boldsymbol{v})\phi(\boldsymbol{v})\, d\boldsymbol{v} \\ &= \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} (f'f'_* - ff_*)(\phi + \phi_* - \phi' - \phi'_*)B\, d\boldsymbol{v}_*\, d\boldsymbol{\sigma}\, d\boldsymbol{v}.\end{aligned}$$

A function $\phi(\boldsymbol{v})$ is called a *collision invariant* if

$$\int_{\mathbb{R}^3} Q(f,f)(\boldsymbol{v})\phi(\boldsymbol{v})\, d\boldsymbol{v} = 0.$$

From expression (2.5) it follows that $\phi(\boldsymbol{v}) = 1$ is a collision invariant, and conservation of momentum and energy imply that $\phi(\boldsymbol{v}) = \boldsymbol{v}$ and $\phi(\boldsymbol{v}) = |\boldsymbol{v}|^2$ are also collision invariants. These collision invariants correspond to respectively, conservation of total mass, total momentum and total energy.

In addition to the collision invariants, Boltzmann also observed that $Q(f,f)(\boldsymbol{v}) = 0$ if and only if

$$\int_{\mathbb{R}^3} Q(f,f)(\boldsymbol{v})\log(f(\boldsymbol{v}))\, d\boldsymbol{v} = 0.$$

The unique solution to this equation is $f(\boldsymbol{v}) = M[f](\boldsymbol{v})$, where

$$M[f](\boldsymbol{v}) = \frac{\rho_f}{(2\pi T_f)^{3/2}} \exp\left(-\frac{|\boldsymbol{v} - \boldsymbol{u}_f|^2}{2T_f}\right),$$

with ρ_f, $\boldsymbol{u}_f$ and T_f denoting respectively the density, mean velocity and temperature of the gas:

$$\begin{aligned}\rho_f &= \int_{\mathbb{R}^3} f(\boldsymbol{v},t)d\boldsymbol{v},\\ \rho_f \boldsymbol{u}_f &= \int_{\mathbb{R}^3} \boldsymbol{v} f(\boldsymbol{v},t)d\boldsymbol{v},\\ 3\rho_f T_f &= \int_{\mathbb{R}^3} |\boldsymbol{v}-\boldsymbol{u}_f|^2 f(\boldsymbol{v},t)d\boldsymbol{v}.\end{aligned}$$

These expressions also make sense in the spatially dependent t case; then the quantities ρ_f, $\boldsymbol{u}_f$ and T_f depend on the spatial variable $\boldsymbol{x}$. The distribution $M[f]$ is called the Maxwellian distribution and describes the velocity distribution of the gas in an equilibrium state.

The H-functional is defined by

$$H[f](t) = \int_{\mathbb{R}^3} f(\boldsymbol{v},t)\log(f(\boldsymbol{v},t))\, d\boldsymbol{v}.$$

Boltzmann proved the celebrated H-theorem which states that, if f is a solution to the Boltzmann equation, then

$$\frac{d}{dt}H[f](t) \le 0.$$

The H-theorem says that the H-functional or entropy is non-increasing with time and that the Maxwellian distribution is the only possible stationary solution to the spatially homogeneous Boltzmann equation. Note that in Physics, the common definition of entropy differs from the one given here by a minus sign.

The H-theorem raised many controversies against Boltzmann because it contradicted the time reversibility of the Newtonian mechanics for a particle system. If one reverses the velocities of all the particles at time $t = T$ and follow their evolution backward, one finds that the particles at $t = 0$ have minus initial velocities. Since the Boltzmann equation is obtained as the number of particles tend to infinity one expects the reversibility property to hold for the Boltzmann equation. But if $f(\boldsymbol{v},t)$ is a solution to the Boltzmann equation, then $f(-\boldsymbol{v},-t)$ is not a solution to the Boltzmann equation. This is referred to as the Loschmidt paradox and seemed to be an obstacle towards the derivation of the Boltzmann equation from the Newton's equations by letting the number of particles tend to infinity. A rigorous mathematical derivation of this was first obtained in 1975 by Lanford [**23**]. However, a drawback with Lanford's result is that it only holds for a short time, a result for a large time scale is still missing. Recent results in this area can found in [**18**], [**28**] and the references therein.

A simplified model used in applications is the so called BGK model introduced by Bhatnagar-Gross-Krook [**1**], which is obtained by replacing the collision integral $Q(f,f)$ in (2.3) by the Maxwellian $M[f]$. The full BGK equation reads

$$\frac{\partial}{\partial t}f + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f = \tau(M[f]-f), \tag{2.6}$$

where $f = f(\boldsymbol{x},\boldsymbol{v},t)$. In this case $M[f]$ is called a local Maxwellian since the quantities ρ_f, $\boldsymbol{u}_f$ and T_f depend on $\boldsymbol{x}$. Since these quantities are computed from f, equation 2.6 is a strongly nonlinear equation. The local Maxwellian $M[f]$ has the same density, mean velocity and temperature as f. The parameter τ depends on the density and temperature of the gas. The BGK equation satisfies the same conservation laws and H-theorem as the Boltzmann equation. An introduction to the BGK model can be found in [**12**].

In this thesis we only consider the spatially homogeneous BGK equation. This equation is given by

$$\frac{\partial}{\partial t}f(\boldsymbol{v},t) = \tau(M[f](\boldsymbol{v}) - f(\boldsymbol{v},t)).$$

Without giving detailed information, we mention that the study of the spatially homogeneous Boltzmann equation has made much progress and is well understood today. A thorough discussion is given in [**32**]. The complete Boltzmann equation (2.2) is less understood and the most general existence theory so far is due to Di Perna and Lions, [**15**]. Uniqueness of these solutions, in the general setting of L^1 solutions is still an open problem.

3. A Probabilistic Approach

In an attempt to understand the validation of the spatially homogeneous Boltzmann equation and the rate at which the solutions converge to equilibrium, the Maxwellian, in a seminal work, Mark Kac [**22**] used a probabilistic approach two answer these equations. Extensive research has been performed to extended the ideas of Kac and answer some of the questions which was left unsolved in his paper. We are now giving a quite rather detailed description of the Kac model since it builds the basis of the contents in the thesis.

4. The Kac Model

The original model that Kac studied is a simple jump process model. Consider N identical particles $v_1, \ldots, v_N$ where, each $v_i \in \mathbb{R}$ represents the one-dimensional velocity of the i-the particle. It is assumed that the total kinetic energy in the system is conserved. The phase space of the particle system is defined to be the sphere in $\mathbb{R}^N$,

$$\mathbb{S}^{N-1}(\sqrt{N}) = \left\{ (v_1, \ldots, v_N) \ : \ \sum_{i=1}^{N} v_i^2 = N \right\} \tag{4.1}$$

Interactions between the particles are described as random collisions involving two particles in such way that the total energy in the system is conserved, the collision process is defined as follows:

(1) For $i \neq j$, choose a pair (v_i, v_j) uniformly among the $\frac{N(N-1)}{2}$ possible pairs.
(2) Choose an angle θ according to an even probability density $b(\theta)$ on the circle. In the original Kac model
$$b(\theta) = \frac{1}{2\pi}.$$
(3) The pair (v_i, v_j) represents a point in the plane $\mathbb{R}^2$, and this point is rotated around the origin with the angle theta. The new pair of velocities (v_i', v_j') are given by
$$\begin{aligned} v_i' &= v_i \cos\theta - v_j \sin\theta, \\ v_j' &= v_j \sin\theta + v_i \cos\theta. \end{aligned}$$

The collision process preserves energy, i.e.,

$$v_i^2 + v_j^2 = v_i'^2 + v_j'^2.$$

With $\boldsymbol{V} = (v_1, \ldots, v_N)$ denoting the state of the system before a collision, the state of the system after a collision involving particle i and j is given by

$$R_{i,j}(\theta)\boldsymbol{V} = (v_1, \ldots, v_{i-1}, v_i', v_{i+1}, \ldots, v_{j-1}, v_j', v_{j+1} \ldots, v_N).$$

In other words, a collision means that the point $\boldsymbol{V}$ jumps to the new point $R_{i,j}(\theta)\boldsymbol{V}$ in phase space. Repeating the steps above describes a random walk on the phase space $\mathbb{S}^{N-1}(\sqrt{N})$. Note that conservation of momentum has been dropped since the velocities are one-dimensional. Requiring both conservation of energy and momentum would lead to the trivial process that either the particles keep their velocities or exchange them.

So far time has not been mentioned. To obtain a complete stochastic process it is assumed that the waiting times T between collisions are independent and exponentially distributed with

$$\mathbb{E}(T) = \frac{1}{N}.$$

Since the exponential distribution has the memoryless property, the stochastic collision process defined above describes a Markov jump process on $\mathbb{S}^{N-1}(\sqrt{N})$. With this choice of T, it follows that as N (number of particles) increases, the number of collisions also increases in such away that the expected number of collisions per coordinate v_j remains constant. For a nice survey and introduction to the Kac model, see [**31**] and the references therein.

To study the Markov process above, Kac considered the *master equation* (Kolmogorov forward equation), describing the time evolution of the probability density on phase space. Assume that the point $\boldsymbol{V}$ initially is distributed according to the probability density $F_N(\boldsymbol{V},0)$ with respect to σ^N, the uniform measure on $\mathbb{S}^{N-1}(\sqrt{N})$. At time t, the density $F_N(\boldsymbol{V},t)$ satisfies the following master equation

$$\frac{\partial}{\partial t}F_N(\boldsymbol{V},t) = \mathscr{K}F_N(\boldsymbol{V},t), \tag{4.2}$$

where

$$\mathscr{K} = N(Q_N - I) \tag{4.3}$$

with

$$Q_N g(V) = \frac{2}{N(N-1)}\sum_{i<j}\int_0^{2\pi} g(R_{i,j}(\theta)\boldsymbol{V})\,\frac{d\theta}{2\pi}. \tag{4.4}$$

A thorough derivation of the master equation (4.2) can be found in [**3**,**5–7**].

The master equation has the expected properties, i.e, conservation of mass and conservation of kinetic energy is fulfilled. To verify this, note that, since σ^N is rotation invariant it follows Q_N is invariant on $\mathbb{S}^{N-1}(\sqrt{N})$ with respect to σ^N. Moreover, by a standard computation it follows that Q_N is self adjoint on $L^2\left(\mathbb{S}^{N-1}(\sqrt{N}), d\sigma^N\right)$. Hence, multiplying equation (4.2) by $|\boldsymbol{V}|^k$ and integrating, it follows that

$$\frac{d}{dt}\int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N(\boldsymbol{V},t)|\boldsymbol{V}|^k \, d\sigma^N = 0 \tag{4.5}$$

for all k. Choosing $k=0$ and $k=2$ corresponds to conservation of mass and conservation of kinetic energy, respectively.

The assumption that all particles are identical is reflected in the fact that the initial probability density should be symmetric with respect to permutations of the variables $v_1 \ldots, v_N$.

Definition 1. A probability density F is said to be symmetric on $\mathbb{S}^{N-1}(\sqrt{N})$ if for any bounded continuous function g on $\mathbb{S}^{N-1}(\sqrt{N})$

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} g(\boldsymbol{V})F(\boldsymbol{V})d\sigma^N = \int_{\mathbb{S}^{N-1}(\sqrt{N})} g(\boldsymbol{V}_e)F(\boldsymbol{V})d\sigma^N,$$

where for any permutation e of $\{1,\ldots,N\}$,

$$\boldsymbol{V}_e = (v_{e(1)},\ldots,v_{e(N)}).$$

It is easy to see that the master equation (4.2) preserves the permutation symmetry.

Towards finding the connection between this particle process and Boltzmann equation, Kac studied the marginal densities of F_N.

Definition 2. For $1 \le k < N$, the k-th marginal $f_k^N(v_1,\ldots,v_k)$ of a symmetric probability density F on $\mathbb{S}^{N-1}(\sqrt{N})$ with respect to σ^N is defined by the expression

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} g(v_1,\ldots,v_k)F(\boldsymbol{V})\, d\sigma^N = \int_{\mathbb{R}^k} g(v_1,\ldots,v_k)f_k^N(v_1,\ldots,v_k)\, dv_1\ldots dv_k,$$

where g is any bounded continuous function on $\mathbb{R}^k$.

A standard computation yields

$$f_k^N(v_1,\dots,v_k) = \sqrt{\frac{N}{N-\sum_{i=1}^k v_i^2}} \int_{\Omega_k} F(\boldsymbol{V})\, d\sigma^k(v_{k+1},\dots,v_N), \tag{4.6}$$

where

$$\Omega_k = \mathbb{S}^{N-1-k}(r), \qquad r = \sqrt{N - \sum_{i=1}^k v_i^2},$$

and σ_k is the uniform measure on Ω_k.

The evolution equation for the first marginal of F_N, f_1^N, is obtained by integrating the master equation (4.2) over Ω_1. This leads to

$$\frac{\partial}{\partial t} f_1^N(v_1,t) = 2 \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} \int_0^{2\pi} \left(f_2^N(v_1', v_2', t) - f_2^N(v_1, v_2, t)\right) \frac{d\theta}{2\pi} dv_2, \tag{4.7}$$

where

$$v_1' = v_1 \cos\theta - v_2 \sin\theta, \qquad v_2' = v_1 \sin\theta + v_2 \cos\theta.$$

Note that the evolution equation for f_1^N is not closed because it depends on f_2^N, and in general, the evolution of f_k^N depends on f_{k+1}^N. However, if $f_2^N(v_1,v_2,t)$ could be approximated by the product $f_1^N(v_1,t) f_1^N(v_2,t)$ then, equation (4.7) would look like the spatially homogeneous Boltzmann equation in one dimension with $b = 1/\pi$. To achieve this, Kac defined the notion of probability densities having the "*Boltzmann property*". In modern language, the Boltzmann property is referred to as probability densities being *chaotic*. The formal definition within the framework of the Kac model is the following

Definition 3. Let f be a given probability density on $\mathbb{R}$ with respect to Lebesgue measure. For each $N \in \mathbb{N}$, let F_N be a probability density on $\mathbb{S}^{N-1}(\sqrt{N})$ with respect to σ^N. Then the family of probability densities $\{F_N\}_{N\in\mathbb{N}}$ is said to be f-chaotic if

(1) For $N \in \mathbb{N}$, F_N is symmetric under permutations of the variables $v_1,\dots,v_N$.
(2) For each fixed $k \in \mathbb{N}$, the k-th marginal $f_k^N(v_1,\dots,v_k)$ of F_N converges to $\prod_{i=1}^k f(v_i)$, as $N \to \infty$. The convergence is in the sense

of weak convergence of measures, that is, for any bounded continuous function $g(v_1,\dots,v_k)$ on $\mathbb{R}^k$,

$$\lim_{N\to\infty}\int_{\mathbb{R}^k} g(v_1,\dots,v_k)f_k^N(v_1,\dots,v_k)\,dv_1\dots dv_k$$
$$=\int_{\mathbb{R}^k} g(v_1,\dots,v_k)\prod_{i=1}^k f(v_i)\,dv_1\dots dv_k.$$

The interpretation of probability densities being chaotic is that, the joint density of the the first k fixed velocities becomes asymptotically independent when the total number of particles tends to infinity.

Note that, so far time has not been mentioned in connection with chaotic probability densities. What Kac wanted to accomplish was to show that the solution to the master equation (4.2) is chaotic. Since the solution only depends on initial data, assuming that initial data is chaotic, one must show that this property is propagated in time under the evolution (4.2). This is called *propagation of chaos*.

One important result in [**22**] by Kac is the proof of propagation of chaos for the master equation:

Theorem 4.1. *Assume that the family of probability densities* $\{F_N(\boldsymbol{V},0)\}_{N\in\mathbb{N}}$ *is* $f(v,0)$*-chaotic. Then, for all* $t>0$*, the family of probability densities* $\{F_N(\boldsymbol{V},t)\}_{N\in\mathbb{N}}$*, that is, the solutions to equation (4.2) is* $f(v,t)$*-chaotic and* $f(v,t)$ *satisfies the Boltzmann-Kac equation*

$$\frac{\partial}{\partial t}f(v,t)=2\int_{\mathbb{R}}\int_0^{2\pi}\left(f(v',t)f(u',t)-f(v,t)f(u,t)\right)\frac{d\theta}{2\pi}du, \tag{4.8}$$

with initial data $f(v,0)$*.*

The proof is based on careful analysis of the self adjoint operator $\mathscr{K}$ defining the right hand side of equation (4.2) and a combinatorial argument. Although, the proof by Kac is powerful it has some important limitations. The fact the collisions involve only two particles being independent of all other particles is important in the analysis of $\mathscr{K}$. In the Kac model the collision kernel $b(\theta)=1/(2\pi)$, this could be replaced by any bounded collision kernel without changing the proof. However, the proof by Kac fails in the case when b also depends on the relative velocities. A detailed proof of Theorem 4.1 compared to the one given by Kac can be found in [**7**].

5. Chaotic probability densities

As we have seen, the rigourous connection between the master equation (4.2) and the Boltzmann-Kac equation (4.8) is available through the notion of chaotic probability densities. We are now going to discuss the question about which probability densities are chaotic. We start with a classical example, [**5**]:

Example 1. Let

$$M(v) = \frac{e^{-\frac{v^2}{2}}}{\sqrt{2\pi}}.$$

Then, the uniform probability density F_N on $\mathbb{S}^{N-1}(\sqrt{N})$ is $M(v)$-chaotic.
To see why this is true, recall that the surface area of the sphere $\mathbb{S}^{N-1}(\sqrt{N})$ in $\mathbb{R}^N$ is given by

$$|\mathbb{S}^{N-1}(\sqrt{N})| = \frac{2\pi^{\frac{N}{2}} N^{\frac{N-1}{2}}}{\Gamma(\frac{N}{2})}.$$

This together with (4.6) imply that, the k-th marginal f_k^N of F_N is given by

$$f_k^N(v_1, \dots, v_k) = \frac{\Gamma(\frac{N}{2})}{N^{\frac{k}{2}}\Gamma(\frac{N-k}{2})} \left(1 - \frac{\sum_{i=1}^k v_i^2}{N}\right)^{\frac{N-k-1}{2}}.$$

Since

$$\lim_{N\to\infty} \frac{\Gamma(\frac{N}{2})}{N^{k/2}\Gamma(\frac{N-k}{2})} = \frac{1}{2^{k/2}},$$

it follows that, for any bounded continuous function g on $\mathbb{R}^k$

$$\lim_{N\to\infty} \int_{\mathbb{R}^k} g(v_1, \dots, v_k) f_k^N(v_1, \dots, v_k)\, dv_1 \dots dv_k$$

(5.1)

$$= \int_{\mathbb{R}^k} g(v_1, \dots, v_k) \frac{1}{(2\pi)^{\frac{k}{2}}} \prod_{i=1}^k e^{-\frac{v_i^2}{2}}\, dv_1 \dots dv_k.$$

In [**22**] Kac described an approach to construct chaotic probability densities on $\mathbb{S}^{N-1}(\sqrt{N})$. Let

$$F_N(v_1,\dots,v_N) = \frac{\prod_{i=1}^N g(v_i)}{\int\limits_{\mathbb{S}^{N-1}(\sqrt{N})} \prod_{i=1}^N g(v_i)\, d\sigma^N}, \tag{5.2}$$

where g is a non-negative function satisfying some integrability conditions. Using the saddle point method, Kac showed that the family $\{F_N\}_{N\in\mathbb{N}}$ is f-chaotic, where

$$f(v) = \frac{e^{-z_0 v^2} g(v)}{\int\limits_{-\infty}^{\infty} e^{-z_0 v^2} g(v)\, dv},$$

and $z_0 > 0$ is the unique solution to the equation

$$\int\limits_{-\infty}^{\infty} e^{-z_0 v^2} g(v)\, dv = \int\limits_{-\infty}^{\infty} v^2 e^{-z_0 v^2} g(v)\, dv.$$

By using a different method compared to Kac, based on a fourth moment condition, Carlen, et al., in [**5**] showed the following:

Theorem 5.1. *Let g be a probability density on $\mathbb{R}$ such that*

$$\int\limits_{\mathbb{R}} v^4 g(v)\, dv < \infty, \qquad \int\limits_{\mathbb{R}} g(v)^p\, dv < \infty$$

for some $p > 1$. Then, the the family $\{F_N\}_{N\in\mathbb{N}}$ with σ^N now denoting the normalized uniform measure on $\mathbb{S}^{N-1}(\sqrt{N})$, is g-chaotic.

For an extension of this result to a geometry for physical collisions, see [**10**]. More information on the study of chaotic probability densities can be found in [**16**], [**30**].

We now state the general definition of chaotic probability densities, and an equivalent useful definition in terms of empirical measures, see e.g., [**30**]. Let E be a locally compact polish (separable and metrizable) space. Let $\mathbf{P}(E)$ denote the space of probability measures on E, and $\mathbf{P}_{sym}(E^N)$ the space of symmetric probability measures on the N-fold product space E^N.

Definition 4. Let $f \in \mathbf{P}(E)$ and $F_N \in \mathbf{P}_{sym}(E^N)$. The family of probability measures $\{F_N\}_{N\in\mathbb{N}}$ is f-chaotic if, for any fixed k and any bounded continuous functions $g_1, \dots, g_k$,

$$\lim_{N\to\infty} \langle F_N, g_1 \otimes \cdots \otimes g_k \otimes \underbrace{1 \otimes \cdots \otimes 1}_{N-k} \rangle = \prod_{i=1}^{k} < f, g_i >, \tag{5.3}$$

where $< f, g >$ denotes the integral of g with respect to the probability measure f.

Condition (5.3) is equivalent to the statement that, the k-th marginal of the probability measure F_N converges weakly to $f^{\otimes k}$ on $\mathbf{P}(E^k)$ as N goes to infinity.

For $\boldsymbol{X} = (x_1, \dots, x_N) \in E^N$, the empirical measure $\mu_{\boldsymbol{X}}^N \in \mathbf{P}(E)$ is defined by

$$\mu_{\boldsymbol{X}}^N = \frac{1}{N} \sum_{i=1}^{N} \delta_{x_i}. \tag{5.4}$$

The next lemma which can be found in [**30**] shows the connection between f-chaotic and the convergence of the empirical measures:

Lemma 5.2. *Let $f \in \boldsymbol{P}(E)$ and $F_N \in \boldsymbol{P}_{sym}(E^N)$. The family of probability measures $\{F_N\}_{N\in\mathbb{N}}$ is f-chaotic if and only if $\mu_{\boldsymbol{X}}^N$ converges in law to f as N goes to infinity.*

We end this section by giving an example of non chaotic families of probability densities, for another interesting example, see [**7**].

Example 2. Let g be a probability density on $\mathbb{R}$, and define

$$F_N(v_1, \dots, v_N) = \frac{1}{N} \sum_{i=1}^{N} g(v_i) \prod_{j\neq i} \delta_N(v_j - v_i). \tag{5.5}$$

where

$$\delta_N(v) = \sqrt{\frac{N}{\pi}} e^{-N|v|^2}.$$

Then, the family $\{F_N\}_{N\in\mathbb{N}}$ is not chaotic.
Note that F_N is a probability density on $\mathbb{R}^N$ which is symmetric under permutations of the variables $v_1, \dots, v_N$. The first marginal $f_1^N(v_1)$ of F_N is given by

$$f_1^N(v_1) = \frac{g(v_1)}{N} + \frac{N-1}{N} \int_{\mathbb{R}} g(v) \delta_N(v - v_1)\, dv.$$

We see that the first marginal converges to $g(v_1)$ when N goes to infinity.

The second marginal $f_2^N(v_1, v_2)$ of F_N is given by

$$\begin{aligned} &f_2^N(v_1, v_2) \\ &= \frac{(g(v_1)+g(v_2))\delta_N(v_2-v_1)}{N} + \frac{N-2}{N}\int_{\mathbb{R}} g(v)\delta_N(v_1-v)\delta_N(v_2-v)\,dv \end{aligned}$$

This shows that it is not possible to express the second marginal as a product of two first marginals when N goes to infinity.

6. Convergence to equilibrium

After proving propagation of chaos for the master equation and deriving the Boltzmann-Kac equation, Kac wanted to relate the rate of convergence to equilibrium of solutions to later equation to the rate of convergence to equilibrium of solutions to the master equation.

The convergence to equilibrium of solutions of the Boltzmann-Kac equation has been studied by several authors, see, e.g., [**8**], [**19**], [**25**]. The equilibrium solution is given by the one-dimensional Maxwellian

$$M(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}.$$

Concerning the master equation, its equilibrium solution is given by the constant function 1 on $\mathbb{S}^{N-1}(\sqrt{N})$ with respect to $\overline{\sigma}^N$, where this measure denotes uniform probability measure on $\mathbb{S}^{N-1}(\sqrt{N})$ induced by σ^N. A detailed proof of this fact can be found in, e.g., [**3**], [**22**]. To compute the rate of convergence to equilibrium, Kac considered the L^2 distance and the *spectral gap* of $-\mathcal{K}$ defined by

$$\Delta_N = \inf\{-\langle g, \mathcal{K} g\rangle \mid < g, 1 >= 0, < g, g >= 1\},$$

where the infimum is over all function $g \in L^2\left(\mathbb{S}^{N-1}(\sqrt{N}), d\overline{\sigma}^N\right)$.

If $F_N(\boldsymbol{V}, t)$ is the solution to the master equation with initial data given by $F_N(\boldsymbol{V}, 0)$, a standard computation (the spectral gap theorem) yields

$$\|F_N(\cdot, t) - 1\|_2 \le e^{-\Delta_N t}\|F_N(\cdot, 0) - 1\|_2.$$

Kac was unable to compute the the exact value of Δ_N and conjectured in [**22**] that

$$\liminf_{N\to\infty} \Delta_N > 0.$$

This conjecture was first proved in 2001 by Janvresse [**21**]. However, her method gives no information about a lower bound for Δ_N. Soon after this, Carlen et al. ([**4**]) were able to compute the exact value of Δ_N for all $N \geq 2$. They showed that

$$\Delta_N = \frac{1}{2}\frac{N+2}{N-1}.$$

Later, in [**9**] this result was extended to a 3 dimensional model including momentum conservation.

The question now is if the proof of Kac's conjecture imply exponential in time converge to equilibrium of solutions to the Boltzmann-Kac equation. The answer is unfortunately negative. Since the last equality implies that $\Delta_N > 1/2$ it follows that

$$\|F(\cdot,t) - 1\|_2 \leq e^{-\frac{t}{2}}\|F(\cdot,0) - 1\|_2. \tag{6.1}$$

While the exponent in the last inequality is uniform in N, the L^2 norm of the initial condition is in general affected by N. Recall that we are interested in chaotic probability densities $F_N(\boldsymbol{V},0)$, That is $F(\boldsymbol{V},0) \approx \prod_{i=1}^N f(v_i)$. These probability densities have in general very large L^2 norm such that

$$\|F(\boldsymbol{V},0)\|_2 \geq C^N$$

where $C > 1$. This shows that the estimate (6.1) works only for a time proportional to N. This destroys the exponential decay in time convergence to equilibrium for the Kac-Boltzmann equation.

In the hope of better estimates, a different approach has been taken by investigating the entropy. In what follows we shall be informal, for details, see [**5**]. If F_N is probability density in $\mathbb{S}^{N-1}(\sqrt{N})$ with respect to $\overline{\sigma}^N$, its entropy is defined as

$$H_N(F_N) = \int_{\mathbb{S}^{N-1}(\sqrt{N})} F(\boldsymbol{V}) \log F(\boldsymbol{V})\, d\overline{\sigma}^N.$$

If $F_N(\boldsymbol{V},t)$ is a solution to the master equation, then

$$\frac{d}{dt}H_N(F_N(\cdot,t)) = \langle \log F_N(\cdot,t), \mathcal{K} F_N(\cdot,t)\rangle .$$

Similarly to the definition of the spectral gap Δ_N, the *entropy production* is defined by

$$\Gamma_N = \inf \frac{-\langle \log g, \mathcal{K} g\rangle}{H_N(g)},$$

where the infimum is taken over all symmetric probability densities g on $\mathbb{S}^{N-1}(\sqrt{N})$ with $H_N(g) < \infty$.

A standard computation leads to

$$H_N(F_N(\cdot,t)) \leq e^{-\Gamma_N t} H_N(F_N(\cdot,0)). \tag{6.2}$$

The main difference between using the entropy instead of the L^2 distance lies in the fact that the entropy is *extensive*, that is, since $F_N(\boldsymbol{V},t)$ is $f(v,t)$-chaotic, for large N,

$$H_N(F_N(\cdot,t)) \approx N H(f(\cdot,t)|M(\cdot)), \tag{6.3}$$

where

$$H(f|M) = \int_{\mathbb{R}} f(v) \log\left(\frac{f(v)}{M(v)}\right) dv.$$

Applying (6.3) to both sides of (6.2), it follows that for large N

$$H(f(\cdot,t)|M(\cdot)) \leq e^{-\Gamma_N t} H(f(\cdot,0)|M(\cdot)).$$

Assuming that $\Gamma_N \geq c > 0$ uniformly in N, and using the Csiszár-Kullback-Liebler-Pinsker inequality, it follows that if $f(v,t)$ satisfies Boltzmann-Kac equation

$$||f(\cdot,t)dv - M(\cdot)dv||_{TV}^2 \leq 2e^{-ct} H(f(\cdot,0)|M(\cdot)), \tag{6.4}$$

where "TV" denotes the total variation norm.

What remains is to obtain the proper lower bound for Γ_N. However, this turns out to be a far more difficult problem compared to the estimate of the spectral gap Δ_N. The best result known so far is

$$\Gamma_N \geq \frac{2}{N-1}.$$

This was proved by Villani [**33**]. Moreover, he conjectured that this bound is essentially sharp, i.e,

$$\Gamma_N = \mathcal{O}(\frac{1}{N}).$$

Unfortunately, this would imply that the time it takes reach equilibrium is still proportional to N. For recent progresses in this direction, see [**5**], [**17**].

7. The master equation and propagation of chaos for physical collision models

In [**22**] Kac also described the master equation approach for Markov processes modelling physical collisions. Here, we follow the approach described in [**26**]. Consider a particle system consisting of N identical particles $\boldsymbol{v}_1,\ldots,\boldsymbol{v}_N$, where each $\boldsymbol{v}_i \in \mathbb{R}^3$ represents the velocity of the i-th particle and each particle has mass $m = 2$. The dynamics between particles are modeled as collisions involving two particles such that the total energy and total momentum of the system is conserved, where, without loss of generality

$$\sum_{i=1}^{N} |\boldsymbol{v}_i|^2 = 3N \quad \text{and} \quad \sum_{i=1}^{N} \boldsymbol{v}_i = 0.$$

Let $\boldsymbol{V} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_N)$ denote the state of the system before a collision. The collision process is defined as follows:

(1) For $i \neq j$, choose a pair $(\boldsymbol{v}_i, \boldsymbol{v}_j)$ uniformly from $\boldsymbol{V}$.

(2) Choose a unit vector $\boldsymbol{\sigma} \in \mathbb{S}^2$ with respect to a probability density $b(\cos\theta_{ij})$, where

$$\cos\theta_{ij} = \left\langle \frac{\boldsymbol{v}_i - \boldsymbol{v}_j}{|\boldsymbol{v}_i - \boldsymbol{v}_j|}, \sigma \right\rangle.$$

(3) After the collision, $\boldsymbol{V}$ is updated to

$$R(\theta_{ij})\boldsymbol{V} = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{i-1}, \boldsymbol{v}'_i, \boldsymbol{v}_{i+1} \ldots, \boldsymbol{v}_{j-1}\boldsymbol{v}'_j, \boldsymbol{v}_{j+1} \ldots, \boldsymbol{v}_N),$$

where

$$\begin{aligned} \boldsymbol{v}'_i &= \frac{\boldsymbol{v}_i + \boldsymbol{v}_j}{2} + \frac{|\boldsymbol{v}_i - \boldsymbol{v}_j|}{2}\boldsymbol{\sigma}, \\ \boldsymbol{v}'_j &= \frac{\boldsymbol{v}_i + \boldsymbol{v}_j}{2} - \frac{|\boldsymbol{v}_i - \boldsymbol{v}_j|}{2}\boldsymbol{\sigma}. \end{aligned} \tag{7.1}$$

Note that

$$|\boldsymbol{v}_i|^2 + |\boldsymbol{v}_j|^2 = |\boldsymbol{v}'_i|^2 + |\boldsymbol{v}'_j|^2 \quad \text{and} \quad \boldsymbol{v}_i + \boldsymbol{v}_j = \boldsymbol{v}'_i + \boldsymbol{v}'_j$$

The waiting time until the next collision in a given pair of particles is assumed to be exponentially distributed with parameter $N\Psi(|v_i - v_j|)$, where Ψ is a non-negative function. Repeating the steps above yields a Markov process on $\mathbb{S}^{3N-2}(\sqrt{3N})$. The evolution of phase space density F_N is given by the following master equation

$$\begin{aligned} &\frac{\partial}{\partial t} F_N(\boldsymbol{V}, t) \\ &= \frac{1}{N} \sum_{i<j} \Psi(|v_i - v_j|) \int_{\mathbb{S}^2} \left(F_N(R(\theta_{ij})\boldsymbol{V}) - F_N(\boldsymbol{V}, t). \right) b(\cos\theta_{ij})\, d\boldsymbol{\sigma}. \end{aligned} \tag{7.2}$$

This master equation is, assuming propagation of chaos, connected to the spatially homogeneous Boltzmann equation

$$\frac{\partial}{\partial t} f(\boldsymbol{v},t) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \Big(f(\boldsymbol{v}',t) f(\boldsymbol{u}',t) - f(\boldsymbol{v},t) f(\boldsymbol{u},t) \Big) B(|\boldsymbol{v}-\boldsymbol{u}|, \cos\theta)\, d\boldsymbol{\sigma}\, d\boldsymbol{u}, \tag{7.3}$$

where

$$B(|\boldsymbol{v}-\boldsymbol{u}|,\cos\theta) = \Gamma(|\boldsymbol{v}-\boldsymbol{u}|) b(\cos\theta), \quad \cos\theta = \left\langle \frac{\boldsymbol{v}-\boldsymbol{u}}{|\boldsymbol{v}-\boldsymbol{u}|}, \sigma \right\rangle,$$

and the velocities $\boldsymbol{v}'$, $\boldsymbol{u}'$ are given by (7.1). Kac's method for proving propagation of chaos works for the master equation (7.2) in the case when $\Psi = 1$ and b is bounded. This corresponds to the case of cut-off maxwellian for the 3-dimensional spatially homogeneous Boltzmann equation (7.3). A different proof this was given by McKean [**24**] in 1967.

The case of hard sphere particles, i.e., $\Psi = |\boldsymbol{v}-\boldsymbol{u}|$, $b = 1$ was first almost solved by Grünbaum [**20**] in 1971 by a different approach. Grünbaum's proof was incomplete since it relied on regularity and stability results for the spatially homogeneous Boltzmann equation which was not known at that time. A complete proof was later given by Sznitman in 1984 using martingale techniques, see [**29**], [**30**]. Recently, the work of Grünbaum has been made fully rigorous and extended to particle systems in which one has jumps, drift and diffusion, [**26**], [**27**].

8. Summary of papers

Here we give brief summaries of the contents of the papers included in the thesis.

8.1. Paper I: Propagation of chaos for the thermostatted Kac master equation. In this paper, we establish propagation of chaos for a particle model in the presence of an external force. Collisions between particles are modeled as in the Kac model with the addition that, between the collisions, the particles are accelerated by an external uniform force field with a Gaussian thermostat.

The force field acts equally on each particle, and to keep the total kinetic energy of the system constant, the Gaussian thermostat absorbs the energy supplied into the system by the force.

As in the Kac model the phase space of the dynamics is the sphere $\mathbb{S}^{N-1}(\sqrt{N})$. If $\boldsymbol{V} = (v_1, \ldots, v_N)$ is a random point on phase space, between collisions, it evolves according to

$$\frac{d}{dt}\boldsymbol{V} = \boldsymbol{F}(\boldsymbol{V}) = E\left(\mathbf{1} - \frac{J(\boldsymbol{V})}{U(\boldsymbol{V})}\boldsymbol{V}\right), \tag{8.1}$$

where $E > 0$, and the quantities $J(\boldsymbol{V})$, $U(\boldsymbol{V})$ represent respectively, the average momentum per particle and the average energy per particle, and are given by

$$\begin{aligned} J(\boldsymbol{V}) &= \frac{1}{N}\sum_{i=1}^{N} v_i, \\ U(\boldsymbol{V}) &= \frac{1}{N}\sum_{i=1}^{N} v_i^2. \end{aligned}$$

The force $\boldsymbol{F}$ is obtained by projecting the field $(E, E, \ldots, E)$ onto tangent plane on $\mathbb{S}^{N-1}(\sqrt{N})$ at the point $\boldsymbol{V}$ It is straightforward to verify that the evolution (8.1) preserves U, as expected.

If the random point $\boldsymbol{V}$ is initially distributed according to a probability density $W_N(\boldsymbol{V}, 0)$, its time evolution is given by the following master equation:

$$\frac{\partial}{\partial t} W_N(\boldsymbol{V}, t) + \nabla_{\boldsymbol{V}} \cdot \big(\boldsymbol{F}(\boldsymbol{V}) W_N(\boldsymbol{V}, t)\big) = \mathscr{K}(W_N)(\boldsymbol{V}, t)) \tag{8.2}$$

where $\mathscr{K}$ is given by (4.3). This equation is known as the thermostatted Kac master equation. The left hand side corresponds to the change of the density in time and under the influence of the force, while the right hand side corresponds to the change of the density due to the collisions. In the absence of the force field $\boldsymbol{F}$, equation (8.2) reduces to the original Kac master equation. More information about equation (8.2) can be found in [**34**].

Assuming that propagation of chaos holds, i.e, the family of solutions $\{W_N(\boldsymbol{V}, t)\}_{N \in \mathbb{N}}$ to equation (8.2) is $f(v, t)$-chaotic, in [**34**] it is shown that $f(v, t)$ satisfies the following equation

$$\frac{\partial}{\partial t} f(v, t) + E \frac{\partial}{\partial v}\big(1 - \xi(t) f(v, t)\big) = Q(f, f), \tag{8.3}$$

where

$$\xi(t) = \int_R v f(v,t)\, dv, \tag{8.4}$$

and

$$Q(f,f)(v) = \int_R \int_0^{2\pi} \big(f(v',t)f(u',t) - f(v,t)f(u,t)\big)\, \frac{d\theta}{2\pi}\, du, \tag{8.5}$$

with $v' = v\cos\theta - u\sin\theta$ and $u' = v\cos\theta + u\sin\theta$.

Kac's proof of propagation of chaos can not be adjusted to show propagation of chaos for the thermostatted Kac master equation. The main difficulty is due to the structure of the force field. Since it depends on all the particles, mainly through $J(\boldsymbol{V})$, during a collision all the particles are present, while in the Kac model the collisions involves only two particles. Unfortunately, the estimates that are needed to verify propagation of chaos fail for the thermostatted Kac master equation.

To justify propagation of chaos, we follow an approach introduced in [**2**]. In this paper propagation of chaos is shown for a particle model with a master equation similar to thermostatted master equation but with a different collision model.

Let us briefly describe the strategy to achieve propagation of chaos in our paper. The first step is to introduce an approximation process to simplify the correlations that are created by force field. Define the quenched current and the quenched energy approximations as

$$\widehat{J}_{W_N}(t) = \frac{1}{N}\sum_{i=1}^{N} < v_i >_{W_N(\boldsymbol{V},t)} \quad \text{and} \quad \widehat{U}_{W_N}(t) = \frac{1}{N}\sum_{i=1}^{N} < v_i^2 >_{W_N(\boldsymbol{V},t)}, \tag{8.6}$$

where $< \cdot >_{W_N}$ denotes the expectation with respect to W_N. We now define the modified force field $\widehat{\boldsymbol{F}}_{W_N}(t)$ by

$$\widehat{\boldsymbol{F}}_{W_N}(t) = E\left(\boldsymbol{1} - \frac{\widehat{J}_N(t)}{\widehat{U}_N(t)}\boldsymbol{V}\right). \tag{8.7}$$

The master equation describing the evolution of phase space density, where the particles collide as in the Kac model and are accelerated between collisions under the influence of the modified force field reads

$$\frac{\partial}{\partial t}\widehat{W}_N(\boldsymbol{V},t)+\nabla\cdot(\widehat{\boldsymbol{F}}_{\widehat{W}_N}(t)\widehat{W}_N(\boldsymbol{V},t))=\mathscr{K}\widehat{W}_N(\boldsymbol{V},t), \tag{8.8}$$

where now the modified force is the one corresponding to the density $\widehat{W}_N(\boldsymbol{V},t)$.

Given initial density $\widehat{W}_N(\boldsymbol{V},0)$, we obtain in Lemma 2.1 that $\widehat{U}_{\widehat{W}_N}(t)$ is constant in time and that $\widehat{J}_{\widehat{W}_N}(t)$ satisfies the following differential equation

$$\frac{d}{dt}\widehat{J}_{\widehat{W}_N}(t)=E-E\frac{\widehat{J}_{\widehat{W}_N}(t)^2}{\widehat{U}_{\widehat{W}_N}(t)}-2\widehat{J}_{\widehat{W}_N}(t). \tag{8.9}$$

The advantage of this approximation process is that the particles evolve independently between collisions. The evolution of the particles between collisions is described by

$$\frac{d}{dt}\widehat{\boldsymbol{V}}=\widehat{\boldsymbol{F}}_{\widehat{W}_N}(t). \tag{8.10}$$

By making a careful analysis and using ideas from [**7**], [**22**], in Theorem 3.1 we obtain a quantitative propagation of chaos result for master equation (8.8). This result is an important step in the direction to adapting the strategy developed in [**2**] for controlling the effects of correlations that are created by the thermostatted force field.

The second step is to make a pathwise comparison between the stochastic process $\boldsymbol{V}(t)$ corresponding to the master equation (8.2), and the stochastic process $\widehat{\boldsymbol{V}}(t)$ corresponding to the master equation (8.8). The main result is in Theorem 4.6 which states that, for all $\epsilon>0$

$$\lim_{N\to\infty}\mathbb{P}\left\{\|\boldsymbol{V}(t)-\widehat{\boldsymbol{V}}(t)\|_N>\epsilon\right\}=0. \tag{8.11}$$

In the last step, we combine Theorem 3.1 and Theorem 4.6 to show propagation of chaos for the thermostatted Kac master equation.

8.2. Paper II: Chaotic distributions for relativistic particles. As we have discussed, in the Kac model the phase space of the dynamics is defined through the conservation of total classical kinetic energy of the particles. The phase space is given by the manifold.

$$\mathbb{S}^{N-1}(\sqrt{N})=\left\{(v_1,\dots,v_N)\ :\ \sum_{i=1}^N v_i^2=N\right\}. \tag{8.12}$$

In this paper we study a modified Kac model. The inspiration comes from the theory of relativity, where the kinetic energy is different from classical kinetic energy. If $\phi(v)$ denotes the kinetic energy of a particle, in a one-dimensional relativistic Kac model where v represents the momentum rather than the velocity of a particle with normalized mass and normalized speed of light, $\phi(v)$ is given by

$$\phi(v) = \sqrt{v^2+1} - 1. \tag{8.13}$$

In the paper we assume that ϕ is an arbitrary function energy function on $\mathbb{R}$ with the natural constraints that ϕ is even, increasing with $\phi(0) = 0$. The dynamics between particles in modified Kac model are the same as in the original Kac model, but the phase space is now given by the manifold

$$\Omega^{N-1}(\sqrt{N}) = \left\{ (v_1, \dots, v_N) \Big| \sum_{i=1}^{N} \phi(v_i) = N \right\}. \tag{8.14}$$

In [**22**] Kac showed that the uniform distribution on $\mathbb{S}^{N-1}(\sqrt{N})$ is $\frac{1}{2\pi} e^{\frac{v^2}{2}}$-chaotic. The main goal of our paper is to investigate chaoticity property of the uniform distribution on $\Omega^{N-1}(\sqrt{N})$. Before stating our main result, the following definition is needed

Definition 5. Let

$$H(v_1, \dots, v_N) = \sum_{i=1}^{N} \phi(v_i). \tag{8.15}$$

Provided that $\|\nabla H\| = 0$, the microcanonical measure $\eta^{(E)}$ on $\Omega^{N-1}(\sqrt{E})$ is defined by

$$\eta^{(E)} \frac{\sigma_\Omega}{\|\nabla H\|}, \tag{8.16}$$

where σ_Ω is the surface measure on $\Omega^{N-1}(\sqrt{E})$.

Note that, on $\mathbb{S}^{N-1}(\sqrt{N})$, the microcanonical measure is directly proportional to the surface measure.

Following Kac's approach to construct chaotic probability densities on $\mathbb{S}^{N-1}(\sqrt{N})$, in Theorem 2.4 we show that the uniform distribution on $\Omega^{N-1}(\sqrt{N})$ with respect to the microcanonical measure is $Ce^{-z_0\phi(v)}$-chaotic, where z_0 is unique real solution to an equation and C is a normalisation constant.

We next explain that propagation of chaos holds for the modified Kac model where the invariant measure is given by the microcanonical measure on $\Omega^{N-1}(\sqrt{N})$. This is an immediate consequence of propagation of chaos for the Kac model.

In the last section, we give a formal description of how one can extend Theorem 2.4 to the case $v \in \mathbb{R}^3$. This case includes conservation of total momentum.

8.3. Paper III: From a particle model to the BGK equation. In section 2 we briefly introduced the BGK equation. This equation is an approximation to the Boltzmann equation by a relaxation model. The nonlinear gain term, i.e., the positive part of the collision integral in the Boltzmann equation is replaced by a Maxwellian which has the same density, macroscopic velocity and temperature as the solutions to the equation.

In section 4 we described the Kac model. This N-particle model is connected to a Boltzmann-like equation in the limit of infinitely many particles. Moreover, this Boltzmann equation has an equilibrium solution given by the Maxwellian

$$\mathscr{M}(v) = \frac{e^{\frac{v^2}{2}}}{\sqrt{2\pi}}.$$

In this paper we construct a particle model which converges to the BGK equation in the limit of infinity many particles. We consider the one-dimensional spatially homogeneous BGK equation

$$\frac{\partial}{\partial t} f(v,t) = \lambda_1 \left(\mathscr{M}(v) - f(v,t) \right), \tag{8.17}$$

where the parameter $\lambda_1 > 0$ and f is a probability density on $\mathbb{R}$ such that it has the same first and second moment as $\mathscr{M}$.

The particle system consists of the one-dimensional velocities of N identical *passive* particles and M identical *active* particles, where it is assumed that there are more passive particles than active particles. The passive and active particles have the same mass and are uniformly distributed in space. Let $V = (v_1, \ldots, v_N)$ denote the set of velocities of the passive particles and $W = (w_1, \ldots, w_M)$ the set of velocities of the active particles. The total energy of the system is conserved and the phase space of the particle system is the sphere on $\mathbb{R}^{N+M}$ with radius $N + M$. Collisions between particles occur only among the active particles with the collisions being modeled as in the Kac model. More precisely, the interactions between particles are:

- Exchange between particles: At exponentially distributed time intervals with mean $\frac{1}{\lambda_1 N}$, a particle v_j is uniformly chosen from V

and exchanged with a particle w_k, uniformly chosen from W. This means that the passive particle v_j becomes active and the active particle w_k becomes passive.

- Collisions between active particles: At exponentially distributed time intervals with mean $\frac{1}{\lambda_2 NM}$, the vector W jumps to $R_{ij}(\theta)W$, see Section 4 for the definition of $R_{ij}(\theta)W$.

This defines a Markov jump process on phase space. The parameter λ_2 and the number of active particles M depend on N. To obtain the one-dimensional spatially homogeneous BGK equation we need to specify the exact dependence between M, N and λ_2. The master equation describing the evolution of phase space density $F(V,W,t)$ is given by

$$\frac{\partial}{\partial t}F(V,W,t) = (L_{NM\lambda_2} + U_{NM\lambda_1})F(V,W,t), \tag{8.18}$$

where

(8.19)

$$L_{NM\lambda_2}F(V,W) = \frac{2N\lambda_2}{M-1}\sum_{1\le j<k\le M}\int_0^{2\pi}\Big(F(V,R_{jk}(\theta)W) - F(V,W)\Big)\ \frac{d\theta}{2\pi},$$

and

$$U_{NM\lambda_1}F(V,W) = \frac{\lambda_1}{M}\sum_{j=1}^{N}\sum_{k=1}^{M}\Big(F(X_{j,k}(V,W)) - F(V,W)\Big), \tag{8.20}$$

with

$$X_{j,k}(V,W) = (v_1,\ldots,v_{j-1},w_k,v_{j+1},\ldots,v_N,w_1,\ldots,w_{k-1},v_j,w_{k+1},\ldots,w_M).$$

The first term in right hand side of equation (2.1) describes the change of F due to the collisions between active particles, and the second term the effect of exchanges between passive and active particles.

We show that the one particle density of a passive particle satisfies the the one-dimensional spatially homogeneous BGK equation when $N \to \infty$. To achieve this, we use the spectral gap formula for the Kac model proved in [**4**]. By increasing the number of collisions, thats choosing λ_2 large enough, the set of active particles will be uniformly distributed on a sphere with radius depending on the energy of the passive particles. This means that when a particle returns to a passive state its distribution is given by the one-particle marginal of the uniform distribution of the sphere with radius depending on the energy of the passive particles. Since the one particle marginal of the uniform distribution on a sphere with radius M converges to the Maxwellian when $M \to \infty$, we expect to obtain the BGK equation when $N \to \infty$. To make this precise we need to specify the exact dependence between M,N and λ_2. We obtain that M and λ_2 satisfy $N/M \to \infty$, $N/M^2 \to 0$ and $\lambda_2 \to \infty$ when $N \to \infty$. Our main result is summarized in Theorem 4.1.

9. Contribution of Dawan Mustafa to the joint papers

For all three papers, the initial formulation of the problem was made by B Wennberg. The authors together contributed to making the ideas precise, and to the mathematical proofs, and in particular in Paper I, the adaptation of E Carlen's ideas in a related paper was essential. In all three papers, the calculations and estimates needed to realize these ideas were carried out by D Mustafa, who also wrote the papers based on the joint efforts.

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