Thesis for the degree of Doctor of Philosophy

Kinetic equations with a Gaussian thermostat

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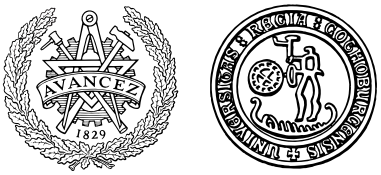

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Abstract

This thesis deals with the mathematical and computational studies of kinetic equations in the presence of an external force field and a Gaussian thermostat. We introduce a stochastic model where particles with one and three-dimensional velocities, in addition to the random collisions, are acted upon by an external force field and in the presence of a Gaussian iso-kinetic thermostat. We derive master equations, which govern the time evolution of the probability distribution of the velocities. Kinetic equations are derived under the assumption of molecular chaos. These equations describe the time evolution of the one-particle distribution function in the limit of infinitely many particles. We also consider the stationary problems.

For the time-dependent thermostatted Kac equation the existence of solutions is established and the time evolution of moments of the solutions are also studied. The non-equilibrium stationary states are treated in further detail. In a particular case, it is shown that, such a state has a singularity. We also discuss a method of constructing asymptotic solutions to the stationary equation.

Numerical simulations using the Monte Carlo method are carried out for both one and three-dimensional velocities. The simulation results, illustrating the main features of the stationary solutions for the respective equations, are presented.

Key words and phrases : Many-particle system, Gaussian iso-kinetic thermostat, Kac's master equation, Kac equation, Boltzmann equation, Non-equilibrium stationary states, Monte Carlo method.

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Contents

Summary

This dissertation comprises four chapters and one published article. It deals with the mathematical and computational studies of kinetic equations in the presence of an external force and a Gaussian thermostat.

The first chapter contains some introductory material. It highlights the essentials of kinetic equations and the mathematical background of deterministic thermostats to motivate our study.

In the second chapter we combine the ideas from chapter one, to derive a Kac-like master equation, which governs the time evolution of probability densities Ψ_N on $\mathbb{S}^{N-1}(\sqrt{N})$:

$$\frac{\partial}{\partial t}\Psi_N \;+\; \nabla\cdot\big(\mathbf{F}\,\Psi_N\big) \;=\; K(\Psi_N).$$

Here $\mathbf{F}$ is a thermostatted force field - obtained by projecting an arbitrary applied field onto the tangent space of $\mathbb{S}^{N-1}(\sqrt{N})$. Physically this corresponds to keeping the kinetic energy constant. The operator K is a linear integral operator acting on pairs of coordinates of Ψ_N and corresponds to the collision operator in the Boltzmann equation.

Assuming molecular chaos a kinetic equation – the thermostatted Kac equation – is derived. It describes the time evolution of the one-particle distribution function in the limit of infinitely many particles and is given by

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

where E denotes the strength of the applied field,

$$\zeta(t) \;=\; \int_{\mathbb{R}} v\,f(v,t)\,dv,$$

and

$$Q(f,f)(v) \;=\; \int_{\mathbb{R}}\int_{-\pi}^{\pi}\Big(f(v',t)f(v'_*,t)-f(v,t)f(v_*,t)\Big)\,\frac{1}{2\pi}\,d\theta\,dv_*.$$

We prove existence of solutions to this equation and study the time evolution of moments of the solutions. The non-equilibrium stationary states for the thermostatted Kac equation are studied in further detail. We show that the stationary solutions of (1) are given by fixed points of the map $f \mapsto \mathcal{A}(f)$ which is defined by

$$\mathcal{A}(f)(v) \;=\; \frac{1}{|v-\kappa|}\int_{\mathbb{R}} \Phi\left(\frac{w-\kappa}{v-\kappa}\right) Q^{+}(f,f)(w)dw,$$

where

$$\Phi(y) \;=\; \frac{\gamma+1}{|y|^{\gamma+1}}\mathbb{1}_{\{y>1\}}(y).$$

It is also proved that, for $E<\sqrt{2}$, $f\in C(\mathbb{R})$; for $E=\sqrt{2}$, f has a logarithmic singularity; and for $E>\sqrt{2}$, f has a power-like singularity. A method of constructing an asymptotic solution to the stationary equation is also considered.

The third chapter contains a related study for the case of three-dimensional velocities. The spatially homogeneous Boltzmann equation is considered in the presence of an external force field and a Gaussian thermostat. Some of the questions that were studied for the Kac case are addressed, although mostly on a formal level. Assuming molecular chaos, the limiting Boltzmann equation is derived:

$$\frac{\partial f}{\partial t} \;+\; div_{\mathbf{v}}\Big(\big(\mathbf{e} \;-\; \zeta_e(t)\,\mathbf{v}\big)f(\mathbf{v},t)\Big) \;=\; Q(f,f)(\mathbf{v},t),$$

where $\mathbf{e}(\mathbf{v})\in\mathbb{R}^3$ denotes the external force field,

$$\zeta_e(t) \;=\; \int_{\mathbb{R}^3} \mathbf{e}\cdot\mathbf{v}\, f(\mathbf{v},t)\, d\mathbf{v},$$

and

$$Q(f,f)(\mathbf{v},t) \;=\; \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \big(f(\mathbf{v}',t)f(\mathbf{v}'_*,t) - f(\mathbf{v},t)f(\mathbf{v}_*,t)\big)B\, d\boldsymbol{\sigma}\, d\mathbf{v}_*,$$

is the usual collision operator with differential cross section B. In this case the stationary state is a Dirac mass.

This thesis also contains computational studies using the Monte Carlo method. This is presented in the fourth chapter. We show detailed simulation results for the one-dimensional thermostatted Kac case and some results for the three-dimensional velocities for the Boltzmann case. These results illustrate the main features of the stationary solutions for the respective equations.

Finally we give some concluding remarks and briefly mention some open problems.

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Chapter 1

Introduction

This chapter contains some background materials. It highlights the essentials of kinetic equations and the mathematical settings of deterministic thermostats to motivate our study.

1.1 The Boltzmann equation

According to classical kinetic theory of rarefied mon-atomic gases, the state of a gas at time $t \geq 0$ is described by the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ of its molecules over the space coordinate $\mathbf{x} \in \mathbb{R}^3$ and the velocity coordinate $\mathbf{v} \in \mathbb{R}^3$. The time evolution of f is governed by the Boltzmann equation

$$\frac{\partial f}{\partial t} \; + \; \mathbf{v} \cdot \nabla_{\mathbf{x}} f \; + \; \nabla_{\mathbf{v}} \cdot \big(\mathbf{F}\, f\big) \; = \; Q(f, f), \tag{1.1}$$

where $\nabla_{\mathbf{x}}$ denotes the gradient of f with respect to $\mathbf{x}$, and $\mathbf{F}$ denotes the force field acting on the particles. In many applications $\mathbf{F}$ is specified in terms of the external force per unit mass: gravitational, electrical or electro-magnetic forces. The dot here stands for the usual Euclidean inner product in $\mathbb{R}^3$.

The collision term on the right hand side of the equation is a nonlinear integral operator and describes the binary collisions involved. The collisions are assumed to be localized in time and space, so that the collision operator acts only on the velocity dependence of the distribution function f. We can write $f(\mathbf{v}) \mapsto Q(f, f)(\mathbf{v})$, where

$$Q(f, f)(\mathbf{v}) \; = \; \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \big(f' f'_* - f f_*\big) B \left(|\mathbf{v} - \mathbf{v}_*|, \frac{\mathbf{v} - \mathbf{v}_*}{|\mathbf{v} - \mathbf{v}_*|} \cdot \boldsymbol{\omega} \right) d\boldsymbol{\omega} d\mathbf{v}_*. \tag{1.2}$$

Here we use the notation $f' = f(\mathbf{v}')$, $f'_* = f(\mathbf{v}'_*)$ and $f_* = f(\mathbf{v}_*)$, where $\mathbf{v}'$ and $\mathbf{v}'_*$ are the post-collisional molecular velocities to the respective pre-collisional molecular velocities $\mathbf{v}$ and $\mathbf{v}_*$. The collisions are assumed to be elastic, so that momentum and kinetic energy are conserved:

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

This gives four constraints on six variables implying that the set of kinematically possible collisions is two dimensional. This may be parameterized by a vector in $\mathbb{S}^2$-the unit sphere in $\mathbb{R}^3$. One such parameterization is

$$\begin{aligned} \mathbf{v}' &= \frac{\mathbf{v}+\mathbf{v}_*}{2} + \frac{|\mathbf{v}-\mathbf{v}_*|}{2}\boldsymbol{\omega} \\ \mathbf{v}'_* &= \frac{\mathbf{v}+\mathbf{v}_*}{2} - \frac{|\mathbf{v}-\mathbf{v}_*|}{2}\boldsymbol{\omega}. \end{aligned} \tag{1.3}$$

In (1.2) $d\boldsymbol{\omega}$ denotes the normalized surface measure on $\mathbb{S}^2$ and $d\mathbf{v}_*$ denotes the Lebesgue measure on $\mathbb{R}^3$. The collision kernel B is a non-negative function whose exact form depends on the physical properties of the gas under study, and thereby on the intermolecular force law which specifies the particular molecular model.

For example, when the intermolecular force varies like $1/r^s$, where r denotes the intermolecular distance and $s > 2$, then the kernel B takes the form

$$B\left(|\mathbf{v}-\mathbf{v}_*|, \cos\theta\right) = |\mathbf{v}-\mathbf{v}_*|^\alpha \, b(\cos\theta). \tag{1.4}$$

Here $\alpha = (s-5)/(s-1)$ and b is a non-elementary function of θ which behaves like $|\theta|^{-\frac{s+1}{s-1}}$, for θ close to 0. The scattering angle θ is defined by

$$\cos\theta = \frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|} \cdot \boldsymbol{\omega}.$$

Since $\frac{s+1}{s-1} > 1$, the singularity in the angular variable θ is always non-integrable. To overcome this difficulty Grad [22] introduced the idea of angular cutoff near $\theta = 0$. This means that b is truncated in such a way that (1.4) is integrable.

In the setting of (1.4) the special case $\alpha = 0$, or equivalently $s = 5$, where the dependence on $|\mathbf{v}-\mathbf{v}_*|$ vanishes, results in what is known as Maxwell molecules.

When the state of the gas is uniform, so that the distribution function is independent of $\mathbf{x}$, (1.1) reduces to the spatially homogeneous Boltzmann equation

$$\frac{\partial f}{\partial t} = Q(f,f), \tag{1.5}$$

or, when there is an external force field

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{v}} \cdot \left(\mathbf{F}\, f\right) = Q(f,f). \tag{1.6}$$

In the remaining part of the thesis, only the spatially homogeneous case is considered.

There is a symmetric bilinear form $Q(f,g)$ associated with the collision integral, namely

$$Q(f,g)(\mathbf{v}) \;=\; \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left(f'\,g'_* + g'\,f'_* - f\,g_* - g\,f_*\right)B\,d\boldsymbol{\omega}\,d\mathbf{v}_*. \tag{1.7}$$

When $g=f$, (1.7) reduces to (1.2). It also holds that $Q(f,g)=Q(g,f)$.

The collision operator possesses fundamental properties which imply the conservation principles. To state some of them, let $\varphi(\mathbf{v})$ be any, sufficiently regular, function. If f and φ are such that the indicated integrals exist, the collision integral $Q(f,f)$ fulfills

$$\int_{\mathbb{R}^3} Q(f,f)(\mathbf{v})\varphi(\mathbf{v})\,d\mathbf{v} \;=\; \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left(\varphi'_* + \varphi' - \varphi_* - \varphi\right)f\,f_*\,B\,d\boldsymbol{\omega}\,d\mathbf{v}_*\,d\mathbf{v}. \tag{1.8}$$

By standard changes of variables, this is equivalent to

$$\int_{\mathbb{R}^3} Q(f,f)(\mathbf{v})\varphi(\mathbf{v})\,d\mathbf{v} \;=\; \frac{1}{4}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left(f'f'_* - ff_*\right)\left(\varphi+\varphi_* - \varphi' - \varphi'_*\right)B\,d\boldsymbol{\omega}\,d\mathbf{v}_*\,d\mathbf{v}.$$

In terms of the distribution function f, the mass, ρ, momentum, $\mathbf{m}$, and energy, $\mathcal{E}$, are given as moments:

$$\begin{pmatrix}\rho\\ \mathbf{m}\\ \mathcal{E}\end{pmatrix} \;=\; \int_{\mathbb{R}^3} f(\mathbf{v})\begin{pmatrix}1\\ \mathbf{v}\\ \frac{1}{2}|\mathbf{v}-\mathbf{m}/\rho|^2\end{pmatrix}d\mathbf{v}.$$

The conservation of mass, momentum and energy at the level of the Boltzmann operator is then recovered by taking $\varphi(\mathbf{v}) = 1, v_i, \frac{1}{2}|\mathbf{v}|^2$ with $i=1,2,3$ in (1.8).

$$\int_{\mathbb{R}^3} Q(f,f)(\mathbf{v})\begin{pmatrix}1\\ v_i\\ \frac{1}{2}|\mathbf{v}|^2\end{pmatrix}d\mathbf{v} \;=\; 0.$$

For an integrable cross section B, i.e. with the angular cutoff assumption of Grad[22], the collision integral (1.2) can be decomposed as $Q = Q^+ - Q^-$, where

$$Q^+(f,f)(\mathbf{v}) \;=\; \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} f(\mathbf{v}')f(\mathbf{v}'_*)\,B\,d\boldsymbol{\omega}\,d\mathbf{v}_*, \tag{1.9}$$

$$Q^-(f,f)(\mathbf{v}) \;=\; \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} f(\mathbf{v})f(\mathbf{v}_*)\,B\,d\boldsymbol{\omega}\,d\mathbf{v}_*. \tag{1.10}$$

For any test function φ it holds that

$$\int_{\mathbb{R}^3}\varphi(\mathbf{v})\,Q^+(f,g)(\mathbf{v})\,d\mathbf{v} \;=\; \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\varphi(\mathbf{v}')\,f(\mathbf{v})\,g(\mathbf{v}_*)\,B\,d\boldsymbol{\omega}\,d\mathbf{v}_*\,d\mathbf{v}. \tag{1.11}$$

From the bilinear structure it also follows that

$$Q^+(f,f) \;-\; Q^+(g,g) \;=\; Q^+(f-g,f) \;+\; Q^+(g,f-g). \tag{1.12}$$

One other property peculiar to the Boltzmann equation is the H-theorem, a result which Boltzmann used to successfully explain the irreversible approach to an equilibrium distribution. Define the functional $H[f]$ by

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

Boltzmann's H-theorem states that for every velocity distribution function f

$$\frac{d}{dt}H[f](t) \;=\; \int_{\mathbb{R}^3} Q(f,f)(\mathbf{v})\,\log f(\mathbf{v},t)\,d\mathbf{v} \;\leq\; 0.$$

This result formally follows from (1.8) with $\varphi(\mathbf{v}) = \log f(\mathbf{v},t)$. It says that the entropy $H[f]$, of any solution f to the Boltzmann equation, is non-increasing with time. Equality holds only for the Maxwellian distribution function $M(\mathbf{v})$, which describes an equilibrium state of the gas. The form of this Maxwellian is

$$M(\mathbf{v}) = \Big(\frac{m}{2\pi kT}\Big)^{\frac{3}{2}} \exp\Big(-\frac{m\,|\mathbf{v}-\mathbf{u}|^2}{2kT}\Big),$$

where m denotes the mass, $\mathbf{u}$ denotes the mean velocity, T denotes the temperature of the gas, and k is the Boltzmann constant.

The Boltzmann equation is thoroughly treated in several books, e.g. [10, 11, 12, 36].

1.2 The Kac model and the Kac equation

The Boltzmann equation can formally be derived as the limit of the evolution of an N-particle system, when $N \to \infty$, in such a way that the mean time between collisions, or more precisely the mean free path, remains constant [28, 34, 11]. There are enormous mathematical difficulties in doing this rigorously, and up to date, there is no derivation that is valid for general initial data or for long time intervals.

To overcome this difficulty Kac [27] introduced a stochastic model that evolves due to the random interactions between pairs of particles. Kac considered a spatially homogeneous 'gas' consisting of N point-particles with one-dimensional velocities $v_i \in \mathbb{R}$, $i = 1, 2, \ldots, N$. At exponentially distributed time intervals a pair of velocities, say v_i and v_j, are selected randomly and are assigned new velocities, v_i' and v_j' respectively, by a random rotation in $\mathbb{R}^2$, i.e.

$$\begin{aligned} v_i' &= v_i\,\cos\theta \;-\; v_j\,\sin\theta \\ v_j' &= v_i\,\sin\theta \;+\; v_j\,\cos\theta. \end{aligned} \tag{1.13}$$

We remark that, in this model the scattering angle θ is chosen from a uniform distribution over $[-\pi, \pi)$. Distributions favoring some collisions over others have also been considered in [17].

We also note that $v_i^2 + v_j^2 = v_i'^2 + v_j'^2$, and thus the total energy, $\sum_{i=1}^N v_i^2$, is conserved in the process. This stochastic model, therefore, defines a jump process on the $(N-1)$–dimensional sphere $\mathbb{S}^{N-1}$, which is normalized to have radius $\sqrt{N}$, and is centered at the origin of $\mathbb{R}^N$. For this process to mimic a system of real particles, one takes the jump frequency, i.e. the rate in the exponential distribution, to be proportional to N.

Let $\mathbf{V} \equiv (v_1, v_2, \ldots, v_N)$, the master vector, denote a point on $\mathbb{S}^{N-1}\big(\sqrt{N}\big)$, and let $\Psi_N(\mathbf{V}, 0)$ denote an initial probability distribution of points on $\mathbb{S}^{N-1}\big(\sqrt{N}\big)$. If each of these points evolve according to the Kac process, then the evolved probability density $\Psi_N(\mathbf{V}, t)$ satisfies

$$\frac{\partial}{\partial t}\Psi_N(\mathbf{V}, t) \;=\; K(\Psi_N)(\mathbf{V}, t), \tag{1.14}$$

where K is the linear operator

$$K(\Psi_N) \;=\; N\big(\tilde{K} - I\big)\big(\Psi_N\big). \tag{1.15}$$

Here I denotes the identity operator, and $\tilde{K}$ is defined by

$$\tilde{K}(\Psi_N)(\mathbf{V}, t) = \binom{N}{2}^{-1} \sum_{1 \le i < j \le N} \frac{1}{2\pi} \int_{-\pi}^{\pi} \Psi_N\big(A_{ij}(\theta)\mathbf{V}, t\big)\, d\theta,$$

where $A_{ij}(\theta)\mathbf{V} = \big(v_1, \ldots, v_i', \ldots, v_j', \ldots, v_N\big)$. Equation (1.14) is known as Kac's master equation.

The Kac model has attracted much interest recently. One example is [9], where the spectral gap of the operator K is computed rigorously. This gives an estimate on the rate of convergence towards the steady state.

The main result in [27] concerns the behavior of the one-particle marginal. Towards stating this result, fix a finite k and define the k-particle marginal f_k^N by

$$f_k^N(v_1, \ldots, v_k, t) \;=\; \int_{\mathbb{S}^{N-1-k}\left(\sqrt{N - \sum_{i=1}^k v_i^2}\right)} \Psi_N(v_1, \ldots, v_k; v_{k+1}, \ldots, v_N, t)\, d\sigma_k, \tag{1.16}$$

where $d\sigma_k = d\sigma_k(v_{k+1}, \ldots, v_N)$ denotes the surface element on $\mathbb{S}^{N-1-k}\big(\sqrt{N - \sum_{i=1}^k v_i^2}\big)$. Special cases are the one-particle marginal f_1^N and the two-particle marginal f_2^N which

are given respectively by

$$f_1^N(v_1,t) = \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} \Psi_N(v_1; v_2, \ldots, v_N, t)\, d\sigma_1, \text{ and} \tag{1.17}$$

$$f_2^N(v_1,v_2,t) = \int_{\mathbb{S}^{N-3}\left(\sqrt{N-v_1^2-v_2^2}\right)} \Psi_N(v_1, v_2; v_3, \ldots, v_N, t)\, d\sigma_2. \tag{1.18}$$

Kac proved rigorously that, under suitable conditions on the initial data, $f_1^N(v_1,t)$ converges, as $N \to \infty$, to a solution $f(v,t)$ of the equation

$$\frac{\partial}{\partial t} f(v,t) \;=\; Q(f,f)(v,t), \tag{1.19}$$

where

$$Q(f,f)(v,t) \;=\; \int_{\mathbb{R}} \int_{-\pi}^{\pi} \Big(f(v',t) f(v'_*,t) - f(v,t) f(v_*,t) \Big) \frac{1}{2\pi}\, d\theta\, dv_*, \tag{1.20}$$

with $v' = v\,\cos\theta - v_*\,\sin\theta$ and $v'_* = v\,\sin\theta + v_*\,\cos\theta$.

Equation (1.19), describing the time evolution of the velocity distribution function f, constitutes the Kac equation which is a one-dimensional caricature of the spatially homogeneous nonlinear Boltzmann equation. Observe that in the Kac equation, mass and energy are conserved, but not momentum. This is a significant difference with the Boltzmann equation, and we will see later that it has an important impact when a thermostatted force field is added.

One assumption in Kac's derivation of the nonlinear Boltzmann equation from a microscopic linear model is that, for each N, the probability density Ψ_N is symmetric in the $v_1, v_2, \ldots, v_N$ variables.

Differentiating both sides of (1.17) with respect to t, and using (1.14) yields

$$\begin{aligned} \partial_t f_1^N(v_1,t) \;&=\; \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} \partial_t \Psi_N(v_1; v_2, \ldots, v_N, t)\, d\sigma_1 \\ &=\; \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} K(\Psi_N)(v_1, v_2, \ldots, v_N, t)\, d\sigma_1. \end{aligned}$$

Evaluating this integral, making use of the symmetry condition on Ψ_N, and using the form of f_2^N as defined in (1.18) gives

$$\partial_t f_1^N(v_1,t) \;=\; \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} \frac{1}{2\pi} \int_{-\pi}^{\pi} \Big(f_2^N(v'_1, v'_2, t) - f_2^N(v_1, v_2, t) \Big)\, d\theta\, dv_2, \tag{1.21}$$

where $v'_1 = v_1\cos\theta - v_2\sin\theta$ and $v'_2 = v_1\sin\theta + v_2\cos\theta$.

This is strongly related to the result in (1.19). Note that instead of $f(v,t)\,f(v_*,t)$ as in (1.20), here we have $f_2^N(v_1,v_2,t)$. An equation for f_2^N would contain f_3^N, etc., and thus (1.21) and the corresponding equations for each of the f_k^N, $k \geq 2$, would not form a closed system of equations unless all of them up to $k = N$ are included.

The central concept in establishing this connection is the notion of propagation of molecular chaos [9, 8, 27, 30, 32, 35]. It deals with the hypothesis that the stochastic independence of two random particles in a many-particle system, persists in time, in the limit of infinitely many particles. The following definition is due to Kac [27].

Definition 1.1. *A family of probability densities $\{\Psi_N\}_{N=1}^{\infty}$ is said to have the Boltzmann property, if*

$$\lim_{N\to\infty} f_k^N(v_1,\ldots,v_k,0) = \prod_{j=1}^{k} \lim_{N\to\infty} f_1^N(v_j,0).$$

This says that, as $N \to \infty$, any fixed finite number of coordinates become independent with the same probability distribution.

The following is the main result in [27] on the propagation in time of molecular chaos:

Theorem 1.1. *If $\Psi_N(v_1,\ldots,v_N,0)$ has the Boltzmann property, then $\Psi_N(v_1,\ldots,v_N,t)$, namely the solution to (1.14), has also the Boltzmann property:*

$$\lim_{N\to\infty} f_k^N(v_1,\ldots,v_k,t) = \prod_{j=1}^{k} \lim_{N\to\infty} f_1^N(v_j,t).$$

As a consequence of Theorem 1.1, Kac proved that $f(v,t) = \lim_{N\to\infty} f_1^N(v_1,t)$ satisfies (1.19).

Looking back to (1.21), the above property then implies that

$$\lim_{N\to\infty} f_2^N(v_1,v_2,t) = \lim_{N\to\infty} f_1^N(v_1,t)\ \lim_{N\to\infty} f_1^N(v_2,t),$$

which in turn makes the evolution equation for the one-particle marginal autonomous but nonlinear.

For the purpose of illustrating the above ideas consider the uniform probability density function given by

$$\Psi_N(\mathbf{V},t) \;=\; \left|\mathbb{S}^{N-1}(\sqrt{N})\right|^{-1}, \tag{1.22}$$

where $|\mathbb{S}^{N-1}(\sqrt{N})|$ denotes the surface measure of the sphere $\mathbb{S}^{N-1}(\sqrt{N})$. The corresponding one-particle marginal is

$$f_1^N(v_1,t) \;=\; \frac{\left(1-v_1^2/N\right)^{(N-3)/2}}{\displaystyle\int_{-\sqrt{N}}^{\sqrt{N}}\left(1-v_1^2/N\right)^{(N-3)/2}dv_1}. \tag{1.23}$$

In the limit $N\to\infty$, this $f_1^N(v_1,t)$ converges to the Maxwellian distribution

$$M(v) \;=\; \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{v^2}{2}\right). \tag{1.24}$$

Here we remark that the constant function given in (1.22) is a stationary solution to the master equation (1.14), and the above Maxwellian distribution $M(v)$ is a stationary solution with unit energy to the Kac equation (1.19).

The two-particle marginal corresponding to the Ψ_N in (1.22) is

$$f_2^N(v_1,v_2,t) \;=\; \frac{\left(1-\left(v_1^2+v_2^2\right)/N\right)^{(N-4)/2}}{\displaystyle\int_{v_1^2+v_2^2<N}\left(1-\left(v_1^2+v_2^2\right)/N\right)^{(N-4)/2}dv_1\,dv_2}. \tag{1.25}$$

We see from (1.25) that the two-particle marginal do not factorize for N finite, i.e. $f_2^N(v_1,v_2,t)\neq f_1^N(v_1,t)\,f_1^N(v_2,t)$. In such a case the velocities are clearly not independent: if $v_2,\ldots,v_N$ are known, then $v_1^2=N-\sum_{i=2}^N v_i^2$. In the limit $N\to\infty$, on the other hand, $f_2^N(v_1,v_2,t)$ tends to (and thereby factorizes to)

$$M_2(v_1,v_2) \;=\; \frac{1}{2\pi}\exp\left(-\frac{v_1^2+v_2^2}{2}\right) \;=\; M(v_1)\,M(v_2). \tag{1.26}$$

This example shows that the stochastic independence of velocities may not be achieved before passing to the limit $N\to\infty$.

A related many-particle system with the more physical three-dimensional velocities is studied in [23, 29, 8]. Let the N velocities be denoted by $\mathbf{v}_1,\mathbf{v}_2,\ldots,\mathbf{v}_N\in\mathbb{R}^3$. Let, at random times, pairs of these velocities, say $\mathbf{v}_i$ and $\mathbf{v}_j$, undergo random 'collisions' and are assigned new velocities, $\mathbf{v}_i'$ and $\mathbf{v}_j'$, according to (1.3). This defines a jump process on the $(3N-1)$-dimensional sphere $\mathbb{S}^{3N-1}$ which is normalized to have radius $\sqrt{N}$. In this case the jumps satisfy $\mathbf{v}_i'+\mathbf{v}_j'=\mathbf{v}_i+\mathbf{v}_j$, in addition to the conservation of energy. One may, thus, consider the jump process to take place on

$$\mathbb{S}^{3N-1}\left(\sqrt{N}\right)\;\cap\;\left\{(\mathbf{v}_1,\mathbf{v}_2,\ldots,\mathbf{v}_N):\sum_{i=1}^N\mathbf{v}_i=const.\right\}.$$

The probability density $\Psi_N(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N; t)$ of the N velocities changes in time due to the random collisions according to the master equation

$$\frac{\partial}{\partial t}\Psi_N \;=\; G(\Psi_N), \tag{1.27}$$

where

$$G(\Psi_N) \;=\; N\,(\tilde{G} - I)(\Psi_N). \tag{1.28}$$

Here I denotes the identity operator, and $\tilde{G}$ is given by

$$\tilde{G}\big(\Psi_N\big)(\mathbf{V}, t) \;=\; \binom{N}{2}^{-1} \sum_{1\le i<j\le N} \frac{1}{4\pi}\int_{\mathbb{S}^2} \Psi_N\big(A_{ij}(\boldsymbol{\omega})\mathbf{V}, t\big)\, d\boldsymbol{\omega},$$

with $A_{ij}(\boldsymbol{\omega})\mathbf{V} = \big(\mathbf{v}_1, \ldots, \mathbf{v}_i', \ldots, \mathbf{v}_j', \ldots, \mathbf{v}_N\big)$ and $\mathbf{v}_i'$ and $\mathbf{v}_j'$ are as in (1.3). Grünbaum[23] proved propagation of chaos in this case, and as a consequence that the Boltzmann equation can be derived in the limit $N \to \infty$. Note that this form of G corresponds to a special case of Maxwellian molecules. Grünbaum[23] considers the more general case of cut-off cross sections.

In general it is not possible to find explicit solutions to the nonlinear Boltzmann equation. This is mainly on account of the quadratic nonlinearity in the collision term. Making some basic assumptions on the collision kernel reduces the complexity and help gain insight into the nature of the solution to the Boltzmann equation. Apart from the equilibrium state, there is only one known case of a particular solution to (1.19) with a special type of initial distribution. This is discussed in [19] and is given by

$$f(v,t) \;=\; \frac{1}{2C^{\frac{3}{2}}}\left(\frac{3}{2}(C-1) + (3-C)\frac{v^2}{C^2}\right)\exp\left(-\frac{v^2}{C}\right), \tag{1.29}$$

where

$$C \equiv C(t) \;=\; 3 \;-\; 2\exp\left(-\frac{\sqrt{\pi}}{16}\,t\right).$$

This special solution is obtained using the symmetry property of the Boltzmann equation for Maxwell molecules. This has been thoroughly investigated by Bobylev in [5]. A class of solutions to a model Boltzmann equation for arbitrary initial conditions is given in [18, 2]. They are given in the form of a series expansion in orthogonal polynomials, the coefficients of which can be determined sequentially from a set of nonlinear moment equations. Related techniques are used to study the Kac equation with a force term in [15, 16].

1.3 Deterministic thermostats

In a system composed of a large number of identical particles, where external effects are neglected, the random collisions between the particles will eventually move the system towards equilibrium. The velocity distribution for such a system is the Maxwellian. If, on the other hand, an external force field acts on the system, it results in the production of heat. The applied field does work on the system thereby moving it away from equilibrium. The excess energy needs to be removed so as to achieve a steady state. There are different methods of accomplishing this. One is by coupling the system to thermal reservoirs where the heat is removed by conduction, radiation or convection to the boundaries. This is done by modeling isothermal reservoirs surrounding the system of interest and let the reservoirs exchange heat with the system.

Another method, which is common in non-equilibrium molecular dynamics simulations, is the use of deterministic thermostats. This technique has been in common use in statistical mechanics as a means of constructing and characterizing steady states of relatively simple but still interesting models of systems which are far from equilibrium.

The use of deterministic thermostats in molecular dynamics simulations was first proposed simultaneously and independently by Hoover[25] and Evans[20]. Both proceed by introducing a damping term into the equations of motion, although in slightly different ways. The damping term is adjusted so as to keep the kinetic energy constant in the former and to keep the internal energy constant in the latter.

This way of thermostatting non-equilibrium molecular dynamics simulations by modifying the equations of motion was put in a theoretical framework when the connection with Gauss' principle of least constraint was established, see for example, Evans et al [21]. This dynamical principle states that a system subject to constraints will follow trajectories which, in the least-square sense, differ minimally from their unconstrained Newtonian counterparts. To this effect, consider a system described by coordinates $\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$, and time t. Suppose that the system is subject to a constraint, the general form of which is

$$g(\mathbf{X}, \dot{\mathbf{X}}, t) \;=\; C, \tag{1.30}$$

where C is a constant. Differentiating both sides of (1.30) with respect to t gives an acceleration dependent constraint equation:

$$\boldsymbol{\lambda}(\mathbf{X}, \dot{\mathbf{X}}, t) \cdot \ddot{\mathbf{X}} \;+\; \beta(\mathbf{X}, \dot{\mathbf{X}}, t) \;=\; 0, \tag{1.31}$$

where

$$\begin{aligned} \boldsymbol{\lambda}(\mathbf{X}, \dot{\mathbf{X}}, t) \;&=\; \frac{\partial g}{\partial \dot{\mathbf{X}}} \\ \beta(\mathbf{X}, \dot{\mathbf{X}}, t) \;&=\; \frac{\partial g}{\partial \mathbf{X}} \cdot \dot{\mathbf{X}} \;+\; \frac{\partial g}{\partial t}. \end{aligned}$$

The constraint in (1.31) imposes a condition on the acceleration vector of particles in the system.

While unconstrained trajectories obeying Newtonian equations(i.e. $\ddot{\mathbf{X}} = \mathbf{F}$) are free to leave the constraint-hypersurface, the constrained trajectories following the equations of motion $\ddot{\mathbf{X}} = \mathbf{F} - \alpha\mathbf{B}$ are prevented from doing so by the application of the additional constraint force $-\alpha\mathbf{B}$ satisfying (1.31):

$$\alpha \;=\; \frac{\mathbf{B}\cdot\ddot{\mathbf{X}} \;+\; \beta}{\mathbf{B}\cdot\mathbf{B}}.$$

For a Gaussian iso-kinetic thermostat where the kinetic energy K_e of the system is constant of the motion, so that $g(\mathbf{X}, \dot{\mathbf{X}}, t) = \dot{\mathbf{X}}^2 - K_e = 0$, the constrained equations of motion are $\ddot{\mathbf{X}} = \mathbf{F} - \alpha\dot{\mathbf{X}}$. This gives

$$\alpha \;=\; \frac{\mathbf{F}\cdot\dot{\mathbf{X}}}{\dot{\mathbf{X}}^2}. \tag{1.32}$$

The subject of deterministic thermostats in connection with non-equilibrium steady states is thoroughly treated in [24, 31, 33, 37]. A review on the development of the thermostat approach in the study of non-equilibrium systems is detailed in [31].

Gaussian iso-kinetic thermostats have also been used in connection with the Lorentz model for conduction in metals [13, 14, 33]. Related studies, both numerical and analytical, of a system where one or several particles are moving in a two-dimensional array of fixed hard disk scatterer under the influence of an electric field, are also made in [6, 7].

Chapter 2

The Kac equation with a Gaussian thermostat

In the original Kac model the system evolves due to the random jumps which correspond to the random interactions between pairs of particles. It is also interesting to study the effect of an external force on the dynamics of the system, in addition to the collisions.

In this chapter we introduce a stochastic model where the particles in the Kac system, in addition to the random collisions, are accelerated by an external uniform force field. The energy supplied into the system is absorbed by a Gaussian thermostat, a term which keeps the total kinetic energy of the system constant. We derive a Kac-like master equation, which governs the time rate of change of the probability distribution of the N-particle velocities. We then derive and study the limiting Boltzmann-like equation which describes the time evolution of the one-particle distribution function in the limit of infinitely many particles. Existence of solutions to this equation are established and the time evolution of moments of the solutions are also investigated. We study the non-equilibrium stationary states in further detail. A method of constructing an asymptotic solution to the stationary problem is presented.

2.1 The master equation

Consider a spatially homogeneous gas consisting of N point-particles with one-dimensional velocities $v_i \in \mathbb{R}$, $i = 1, 2, \ldots, N$. We modify the original stochastic model by incorporating an external uniform force field $\mathbf{E} = E(1, 1, \ldots, 1) \in \mathbb{R}^N$ which accelerates the

particles between the collisions. This field is supposed to be acting equally on each particle, but in order to keep the total energy constant, it must then be projected onto the tangent plane to the energy surface $S^{N-1}(\sqrt{N})$ at the point $\mathbf{V}$. More precisely, between collisions, the master vector $\mathbf{V} = (v_1, v_2, \ldots, v_N)$ evolves according to

$$\frac{d\mathbf{V}}{dt} \;=\; \mathbf{E} - \frac{\mathbf{E}\cdot\mathbf{V}}{|\mathbf{V}|^2}\mathbf{V}. \tag{2.1}$$

Because of the relatively simple form of this system, the trajectories of $\mathbf{V}$ can be computed explicitly. This is presented and is used in the numerical simulation part.

Let $\Psi_N(\mathbf{V}, t)$ be the probability density of the N-velocities at time t. The unique solution to (2.1) with a given initial data $\mathbf{V}_0$ defines an evolution operator T^t such that $\mathbf{V} = T^t\mathbf{V}_0$. For a fixed t, the map $\mathbf{V}_0 \mapsto \mathbf{V}$ defines a change of variables, and if we denote its Jacobian determinant by $\jmath$, we get the condition that $\partial_t\big(\Psi_N(\mathbf{V}(t,\mathbf{V}_0),t)\,\jmath\big) = 0$, which in turn, since $\jmath \neq 0$, gives

$$\frac{\partial}{\partial t}\Psi_N \;+\; \nabla\Psi_N\cdot\frac{d\mathbf{V}}{dt} \;+\; \Psi_N\frac{1}{\jmath}\frac{\partial\jmath}{\partial t} \;=\; 0. \tag{2.2}$$

To further explore the coupling to the dynamics in (2.1) we introduce the quantities $J(t)$ and $U(t)$ as

$$J(t) \;=\; \frac{1}{N}\sum_{i=1}^{N} v_i(t), \tag{2.3}$$

$$U(t) \;=\; \frac{1}{N}\sum_{i=1}^{N} v_i(t)^2. \tag{2.4}$$

It is easily verified that $U(t)$ is constant, as it should be. We therefore set, without loss of generality, $U = 1$, which is in accordance with taking $\mathbf{V} \in \mathbb{S}^{N-1}(\sqrt{N})$.

Then (2.1), written component-wise, becomes

$$\frac{dv_i(t)}{dt} \;=\; E\left(1 - \frac{J}{U}v_i(t)\right),\; i = 1, 2, 3, \ldots, N. \tag{2.5}$$

This leads us to denote the vector field in the right hand side of (2.1) by $\mathbf{F} \equiv \mathbf{F}(\mathbf{V})$, where

$$\mathbf{F} \;=\; E\left(\mathbf{1} - \frac{J}{U}\mathbf{V}\right) \;=\; E\left(1 - \frac{J}{U}v_1, \ldots, 1 - \frac{J}{U}v_N\right), \tag{2.6}$$

and $\mathbf{1} = (1, 1, \ldots, 1) \in \mathbb{R}^N$. With this we can rewrite (2.2) as

$$\frac{\partial}{\partial t}\Psi_N \;+\; \nabla\Psi_N\cdot\mathbf{F} \;+\; \Psi_N\nabla\cdot\mathbf{F} \;=\; 0.$$

This takes the form of the continuity equation

$$\frac{\partial}{\partial t}\Psi_N \;+\; \nabla\cdot\big(\mathbf{F}\,\Psi_N\big) \;=\; 0,$$

and says that the number of particles is conserved.

We remark that, $\mathbf{F}$ can also be expressed in the form

$$\mathbf{F} \;=\; E\,N\,\sqrt{U}\,\nabla\left(\frac{J}{\sqrt{U}}\right),$$

which shows that, $\mathbf{F}$ is tangent to the sphere $\mathbb{S}^{N-1}(\sqrt{N})$, since $J/\sqrt{U}$ is homogeneous of degree 0.

Until now the dynamics was due only to the driving field $\mathbf{F}$. If we further allow velocity jumps to occur just like in the Kac model, then the probability density Ψ_N will evolve in time according to

$$\frac{\partial}{\partial t}\Psi_N \;+\; E\,\nabla\cdot\big(\mathbf{F}\,\Psi_N\big) \;=\; K(\Psi_N). \tag{2.7}$$

Here $\mathbf{F}$ is as in (2.6) and K is the same collision term as in Kac's original model, i.e.

$$K(\Psi_N)(\mathbf{V},t) \;=\; \frac{2}{N-1}\sum_{1\le i<j\le N}\frac{1}{2\pi}\int_{-\pi}^{\pi}\big(\Psi_N(A_{ij}(\theta)\mathbf{V},t)-\Psi_N(\mathbf{V},t)\big)d\theta,$$

with

$$A_{ij}(\theta)\mathbf{V} \;=\; (v_1,\ldots,v_i\cos\theta-v_j\sin\theta,\ldots,v_i\sin\theta+v_j\cos\theta,\ldots,v_N).$$

Equation (2.7) constitutes a Kac-like master equation.

2.2 The limiting Boltzmann equation

In this section we pass to the limit $N\to\infty$, to derive a Kac equation to f – the limit of the one-particle marginals of the probability densities Ψ_N. Note that because we have assumed $U=1$ in the previous section, we necessarily have $\int_{\mathbb{R}} v^2 f(v,t)dv = 1$.

Theorem 2.1. *Suppose that $\Psi_N(v_1,\ldots,v_N,t)$ is a sequence of C^1-solutions to (2.7) and that Ψ_N is symmetric in the variables $v_1,\ldots,v_N$. If Ψ_N has the Boltzmann property, and if further*

$$f(v,t) \;=\; \lim_{N\to\infty} f_1^N(v,t),$$

exists, then f satisfies the equation

$$\frac{\partial}{\partial t} f \;+\; E\,\frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\,v\big)\,f\Big) \;=\; Q(f,f), \tag{2.8}$$

where

$$\zeta(t) \;=\; \int_{\mathbb{R}} v\,f(v,t)\,dv, \tag{2.9}$$

and

$$Q(f,f)(v) \;=\; \int_{\mathbb{R}}\int_{-\pi}^{\pi}\Big(f(v',t)f(v'_*,t)-f(v,t)f(v_*,t)\Big)\,\frac{1}{2\pi}\,d\theta\,dv_*. \tag{2.10}$$

Notation. In the sequel, for the sake of simplicity, we denote the sphere $\mathbb{S}^{N-1}\big(\sqrt{N}\big)$ by Ω_0, $\mathbb{S}^{N-2}\big(\sqrt{N-v_1^2}\big)$ by Ω_1, and $\mathbb{S}^{N-3}\big(\sqrt{N-v_1^2-v_2^2}\big)$ by Ω_2. Let $d\sigma_0$, $d\sigma_1$, and $d\sigma_2$ denote the surface elements on Ω_0, Ω_1, and Ω_2 respectively.

Proof of Theorem 2.1. Consider the one-particle marginal f_1^N and the two-particle marginal f_2^N which are special cases of the k-particle marginal f_k^N defined in (1.16), namely

$$\begin{aligned} f_1^N(v_1,t) \;&=\; \int_{\Omega_1} \Psi_N(v_1;v_2,\ldots,v_N,t)\;d\sigma_1,\\ f_2^N(v_1,v_2,t) \;&=\; \int_{\Omega_2} \Psi_N(v_1,v_2;v_3,\ldots,v_N,t)\;d\sigma_2. \end{aligned}$$

Differentiating $f_1^N(v_1,t)$ with respect to t and using (2.7) we have that

$$\begin{aligned} \frac{\partial}{\partial t} f_1^N(v_1,t) \;&=\; \int_{\Omega_1} \frac{\partial}{\partial t}\Psi_N(v_1;v_2,\ldots,v_N,t)\,d\sigma_1\\ &=\; -\,E\int_{\Omega_1} \nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\sigma_1 \;+\; \int_{\Omega_1} K(\Psi_N)\,d\sigma_1. \end{aligned}$$

This in turn can be written as

$$\frac{\partial}{\partial t} f_1^N(v_1,t) \;+\; E\int_{\Omega_1} \nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\sigma_1 \;=\; \int_{\Omega_1} K(\Psi_N)\,d\sigma_1. \tag{2.11}$$

We recall Kac's result (see Section 1.2) that, in the limit $N\to\infty$, the integral in the right hand side of (2.11) takes the form of $Q(f,f)$ as given in (2.10). We need to *assume* that this also holds in the present case. Then the rest of the proof follows through the result of Lemma 2.1, which is stated and proved below. ■

Lemma 2.1. *Let the densities $\Psi_N(v_1,\dots,v_N,t)$ be as specified in Theorem 2.1. Let $\zeta(t)$ be as defined in (2.9), and $\mathbf{F}$ as given in (2.6). Then, in the limit $N\to\infty$, we have that*

$$\int_{\Omega_1} \nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\sigma_1 \;\to\; \frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\,v_1\big)f\Big).$$

Proof : Let $\varphi\in C_0^1(\mathbb{R})$ be such that $\varphi=\varphi(v_1)$, and let $\eta_r=\eta_r(|\mathbf{V}|)$. This η_r will later be taken to be an approximation to $\mathbf{1}_{|\mathbf{V}|<r}$, the characteristic function of the ball $\{\mathbf{V}:|\mathbf{V}|<r\}$.

Since η_r is radial we have $\nabla\eta_r\cdot\mathbf{F}=0$. We also have that

$$\nabla\varphi\cdot\mathbf{F} \;=\; \frac{\partial\varphi}{\partial v_1}\left(1-\frac{J}{U}v_1\right).$$

Then we continue by noting that,

$$\int_{\Omega_0}\varphi\,\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)\;d\sigma_0 \;=\; \int_{-\sqrt{N}}^{\sqrt{N}}\varphi\;\left[\sqrt{\frac{N}{N-v_1^2}}\;\int_{\Omega_1}\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)d\sigma_1\right]dv_1.$$

Since we are interested in the limit $N\to\infty$ there is no restriction in assuming that $supp\,(\varphi)\subset[-\sqrt{N},\sqrt{N}]$, and hence the above integral can be written as

$$\int_{\mathbb{R}}\varphi\,\sqrt{\frac{N}{N-v_1^2}}\;\int_{\Omega_1}\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)\,d\sigma_1\,dv_1. \tag{2.12}$$

Formally, if $\eta_r=\mathbf{1}_{|\mathbf{V}|<r}$,

$$\int_{\Omega_0}\varphi\,\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)d\sigma_0 \;=\; \frac{d}{dr}\left(\int_{\mathbb{R}^N}\eta_r\;\varphi\;\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)d\mathbf{V}\right)\Big|_{r=\sqrt{N}}.$$

In the calculations that follow, we assume that η_r is smooth, and then we conclude, by letting η_r converge to the characteristic function. Integration by parts gives

$$\begin{aligned}\int_{\mathbb{R}^N}\eta_r\;\varphi\;\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)d\mathbf{V} \;&=\; -\int_{\mathbb{R}^N}\nabla\big(\eta_r\;\varphi\big)\cdot\big(\mathbf{F}\;\Psi_N\big)d\mathbf{V}\\ &=\; -\int_{\mathbb{R}^N}\varphi\;\nabla\eta_r\cdot\big(\mathbf{F}\;\Psi_N\big)d\mathbf{V}-\int_{\mathbb{R}^N}\eta_r\nabla\varphi\cdot\big(\mathbf{F}\;\Psi_N\big)d\mathbf{V}.\end{aligned}$$

Using the fact that $\nabla\eta_r\cdot\mathbf{F}=0$ and that φ depends only on v_1 the above sum reduces to

$$-\int_{\mathbb{R}}\frac{\partial\varphi}{\partial v_1}\left(\int_{\mathbb{R}^{N-1}}\eta_r\left(1-\frac{J}{U}v_1\right)\Psi_N dv_2\cdots dv_N\right)dv_1.$$

We may assume $supp\,(\varphi) \subset (-r, r)$ because eventually we will set $r = \sqrt{N}$. Then this integral equals

$$-\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \left[\int_0^{\sqrt{r^2 - v_1^2}} \left(\int_{\mathbb{S}^{N-2}(\rho)} \left(1 - \frac{J}{U} v_1\right) \Psi_N \, d\sigma_1 \right) d\rho \right] dv_1,$$

where $\rho \widetilde{\boldsymbol{w}} = (v_2, \ldots, v_N)$, with $\widetilde{\boldsymbol{w}} = (w_2, \ldots, w_N) \in \mathbb{S}^{N-2}$ and $\rho > 0$, makes this integral to take the form

$$-\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \left[\int_0^{\sqrt{r^2 - v_1^2}} \int_{\mathbb{S}^{N-2}(1)} \left[1 - \frac{v_1 + \rho\, \widetilde{\boldsymbol{w}} \cdot \mathbf{1}}{v_1^2 + \rho^2} v_1 \right] \Psi_N(v_1; \rho \widetilde{\boldsymbol{w}})\, \rho^{N-2}\, d\widetilde{\boldsymbol{w}}\, d\rho \right] dv_1.$$

Differentiating this with respect to r gives

$$-\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \frac{r}{\sqrt{r^2 - v_1^2}} \int_{\mathbb{S}^{N-2}(1)} \left[1 - \frac{v_1 + \sqrt{r^2 - v_1^2}\, \widetilde{\boldsymbol{w}} \cdot \mathbf{1}}{r^2} v_1 \right] \left[r^2 - v_1^2\right]^{\frac{N-2}{2}} \Psi_N \, d\widetilde{\boldsymbol{w}}\, dv_1.$$

Setting $r = \sqrt{N}$ and expressing the integral in terms of $d\sigma_1$ rather than the $d\widetilde{\boldsymbol{w}}$ on $\mathbb{S}^{N-2}$ gives

$$-\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \frac{\sqrt{N}}{\sqrt{N - v_1^2}} \int_{\Omega_1} \left(1 - \frac{J}{U} v_1\right) \Psi_N \, d\sigma_1\, dv_1.$$

We prove in Lemma 2.2 below that

$$-\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \frac{\sqrt{N}}{\sqrt{N - v_1^2}} \int_{\Omega_1} \left(1 - \frac{J}{U} v_1\right) \Psi_N \, d\sigma_1\, dv_1 \;\to\; -\int_{\mathbb{R}} \frac{\partial \varphi}{\partial v_1} \Big(\big(1 - \zeta(t)\, v_1\big)\, f \Big)\, dv_1,$$

when $N \to \infty$, and after integration by parts this is

$$\int_{\mathbb{R}} \varphi\, \frac{\partial}{\partial v_1} \Big(\big(1 - \zeta(t)\, v_1\big)\, f \Big)\, dv_1.$$

Comparing this with (2.12) gives the desired result because φ is arbitrary. ■

Lemma 2.2. *Let the densities $\Psi_N(v_1, \ldots, v_N, t)$ be as specified in Theorem 2.1 and let $\zeta(t)$ be as defined in (2.9). Then, in the limit $N \to \infty$, we have that*

$$\int_{\Omega_1} \left(1 - \frac{J}{U} v_1\right) \Psi_N \, d\sigma_1 \;\to\; \big(1 - \zeta(t) v_1\big) f(v_1, t). \tag{2.13}$$

Proof : We start by noting that

$$\begin{aligned} \int_{\Omega_1} \left(1 - \frac{J}{U} v_1\right) \Psi_N \, d\sigma_1 \;&=\; \int_{\Omega_1} \Psi_N \; d\sigma_1 \;-\; v_1 \int_{\Omega_1} \frac{J}{U}\, \Psi_N \, d\sigma_1 \\ &=\; f_1^N \;-\; v_1 \int_{\Omega_1} \frac{J}{U}\, \Psi_N \, d\sigma_1. \end{aligned} \tag{2.14}$$

Next, we use the definition of J, the symmetry condition on Ψ_N, and the condition that the energy is kept constant at 1, to further simplify the integral in (2.14) as

$$\begin{aligned}\int_{\Omega_1} \frac{J}{U}\,\Psi_N\,d\sigma_1 &= \frac{1}{N}\int_{\Omega_1}\frac{v_1}{U}\,\Psi_N\,d\sigma_1 \;+\; \frac{1}{N}\int_{\Omega_1}\frac{v_2+\cdots+v_N}{U}\,\Psi_N\,d\sigma_1\\ &= \frac{1}{N}\,v_1\,f_1^N \;+\; \frac{N-1}{N}\int_{\Omega_1} v_2\,\Psi_N\,d\sigma_1. \end{aligned} \tag{2.15}$$

We write the integral in (2.15) as an iterated integral

$$\begin{aligned}\int_{\Omega_1} v_2\,\Psi_N\,d\sigma_1 &= \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\left[\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\int_{\Omega_2}\Psi_N(v_1,v_2;v_3,\ldots,v_N,t)d\sigma_2\right]dv_2\\ &= \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\,\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\;f_2^N(v_1,v_2,t)\,dv_2. \end{aligned} \tag{2.16}$$

By assumption, Ψ_N has the Boltzmann property, and hence

$$f_2^N(v_1,v_2,t) \;\to\; f_1(v_1,t)\,f_1(v_2,t),$$

as $N\to\infty$. We use this and rewrite the integral in (2.16) as

$$\begin{aligned}&\int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2 f_1^N(v_1,t) f_1^N(v_2,t)dv_2 \;+\\ &+\;\int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\;\left[\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\;f_2^N(v_1,v_2,t)-f_1^N(v_1,t)\,f_1^N(v_2,t)\right]dv_2. \end{aligned} \tag{2.17}$$

Because of our assumption, the functions f_k^N decay sufficiently fast that passing to the limit ($N\to\infty$), the integral in (2.16) converges to $f(v,t)\int_{-\infty}^{\infty} v\,f(v,t)\,dv$. By combining (2.16), (2.15), and (2.14); letting $N\to\infty$, we conclude that

$$\int_{\Omega_1}\left(1-\frac{J}{U}v_1\right)\Psi_N\,d\sigma_1 \;\to\; \big(1-\zeta(t)\,v_1\big)f(v_1,t).$$

■

2.3 On the existence of solutions

In this section we examine the conditions under which a non-negative solution to the time-dependent thermostatted Kac equation exists.

Given a non-negative f_0 we study the following initial value problem

$$\frac{\partial}{\partial t} f \;+\; E \frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\,v\big) f\Big) \;=\; Q(f,f), \quad (t>0) \tag{2.18}$$

$$f(v,0) \;=\; f_0(v), \tag{2.19}$$

$$\zeta(t) \;=\; \int_{\mathbb{R}} v\, f(v,t)\, dv. \tag{2.20}$$

Theorem 2.2. *Let a non-negative f_0 with $\int_{\mathbb{R}} f_0(v)dv = 1$ be given. Then there exists a non-negative $f \in C\left((0,\infty); L^1(\mathbb{R})\right)$ – mild solution to the initial value problem (2.18)-(2.20) and such that $\int_{\mathbb{R}} f(v,t)dv = 1$.*

Remark 2.1. *With initial datum f_0 as in Theorem 2.2 one can not hope for a strong solution in the sense of a C^1–function. For such a strong solution to exist one needs to assume that $f_0 \in W^{1,1}$.*

We start by stating and justifying some preliminary results on the time evolution and the exact form of the current $\zeta(t)$.

Lemma 2.3. *Let a non-negative f_0 with $\int_{\mathbb{R}} f_0(v)dv = 1$ be given. Assume that there exists a non-negative f, solution to the initial value problem (2.18)-(2.20) such that $\int_{\mathbb{R}} f(v,t)\, dv = 1$, and $|v|f(v,t) \to 0$ as $|v| \to \infty$, for each $t \geq 0$. Then $\zeta(t)$ fulfills*

$$\frac{d}{dt}\zeta(t) \;=\; E\,\left(1-\zeta(t)^2\right) - \zeta(t), \tag{2.21}$$

$$\zeta(0) \;=\; \zeta_0 \;\equiv\; \int_{\mathbb{R}} v f_0(v) dv.$$

This can be solved explicitly as

$$\zeta(t) \;=\; \frac{\zeta_+ \;-\; \zeta_-\, C\, e^{-\sqrt{1+4E^2}\,t}}{1 \;-\; C\, e^{-\sqrt{1+4E^2}\,t}}, \tag{2.22}$$

where

$$\zeta_\pm \;=\; \frac{2E}{1 \pm \sqrt{1+4E^2}}, \tag{2.23}$$

and

$$C \;=\; \frac{\zeta_+ \;-\; \zeta_0}{\zeta_- \;-\; \zeta_0}.$$

Proof. First we note that, the collision term Q, as given in (2.10), can be written as

$$Q(f,f)(v,t) \;=\; Q^+(f,f)(v,t) \;-\; f(v,t).$$

Multiplying both sides of this by v, integrating the resulting expression over $\mathbb{R}$ with respect to v, and noting that

$$\int_{\mathbb{R}} v\, Q^+(f,f)(v,t)\, dv \;=\; \int_{\mathbb{R}} v'\, Q^+(f,f)(v,t)\, dv \;=\; 0,$$

we find that

$$\int_{\mathbb{R}} v\, Q(f,f)(v,t)\, dv \;=\; \int_{\mathbb{R}} v\, Q^+(f,f)(v,t)\, dv \;-\; \int_{\mathbb{R}} v\, f(v,t)\, dv \;=\; -\zeta(t). \tag{2.24}$$

Next, from the definition of $\zeta(t)$, it follows that

$$\frac{d}{dt}\zeta(t) \;=\; \int_{\mathbb{R}} v\, \frac{\partial}{\partial t} f(v,t)\, dv.$$

We then use (2.18) to rewrite the the right hand side of the above as

$$\int_{\mathbb{R}} v\, Q(f,f)(v,t)\, dv \;-\; E \int_{\mathbb{R}} v\, \frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\, v\big)\, f(v,t)\Big)\, dv.$$

Noting the result in (2.24) and performing integration by parts gives the form of the differential equation as stated in (2.21).

If $\zeta(0) = \zeta_+$ or $\zeta(0) = \zeta_-$ then $\zeta(t) = \zeta(0)$ for all $t > 0$. Otherwise, the unique solution to the first order non-linear differential equation (2.21) is obtained to be (2.22). ■

In (2.22) we see that the magnitude of the external force E appears as a parameter. Further, as $t \to \infty$ the current $\zeta(t) \to \zeta_+$ independent of the initial data ζ_0. In Figure 2.1 we plot the time evolution of $\zeta(t)$ as given in (2.22) with $E = \sqrt{2}$ and with some values of the initial data $\zeta(0)$ varying between -1 and $+1$.

Next we study the initial value problem

$$\frac{\partial}{\partial t} f \;+\; E\, \frac{\partial}{\partial v}\Big(\big(1-\bar{\zeta}(t)\, v\big) f\Big) \;=\; Q(f,f), \quad (t>0), \tag{2.25}$$

$$f(v,0) \;=\; f_0(v), \tag{2.26}$$

$$\bar{\zeta}(t) \;=\; \frac{\zeta_+ - \zeta_-\, C\, e^{-\sqrt{1+4E^2}\, t}}{1 - C\, e^{-\sqrt{1+4E^2}\, t}}. \tag{2.27}$$

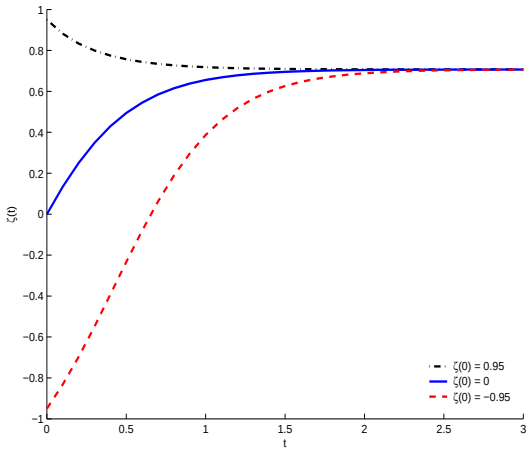

Figure 2.1: The evolution of $\zeta(t)$ according to (2.22) with initial data $\zeta(0) = -0.95, 0, 0.95$, $(E = \sqrt{2})$.

This is exactly like (2.18)–(2.20) except that $\zeta(t) = \int_{\mathbb{R}} v f(v,t) dv$ is replaced by the known function $\bar{\zeta}(t)$.

Towards stating and proving the result on existence and uniqueness of solution to (2.25)–(2.27) we first rewrite (2.25) as

$$\frac{\partial}{\partial t} f \;+\; E\big(1 - \bar{\zeta}(t)\, v\big)\frac{\partial}{\partial v} f \;+\; \big(1 - E\,\bar{\zeta}(t)\, v\big) f \;=\; Q^+(f,f), \tag{2.28}$$

where

$$Q^+(f,f)(v,t) \;=\; \int_{\mathbb{R}} \int_{-\pi}^{\pi} f(v',t) f(v'_*,t) \frac{1}{2\pi}\, d\theta\, dv_*.$$

This constitutes a first-order semilinear equation. We solve this by the method of characteristics and perform an iteration scheme in line with Arkeryd[1].

After integration along characteristics (2.28) becomes

$$\frac{d}{dt} f^{\#} \;+\; \big(1 - E\,\bar{\zeta}(t)\big) f^{\#} \;=\; Q^+(f,f)^{\#}, \tag{2.29}$$

where, for each $v \in \mathbb{R}$, we use the notation

$$f^{\#}(v,t) \;=\; f\big(V(v,t),t\big),$$
$$Q^+(f,f)^{\#}(v,t) \;=\; Q^+(f,f)(V(v,t),t).$$

Here we make use of the transformation

$$V(v,t) \;=\; v\,e^{-\lambda(t)} \;+\; E\,e^{-\lambda(t)}\int_0^t e^{\lambda(s)}\,ds, \tag{2.30}$$

with

$$\lambda(t) \;=\; E\int_0^t \bar{\zeta}(s)ds.$$

The Jacobian of the transformation in (2.30) is $J = e^{-\lambda(t)} > 0$. That J doesn't vanish makes it possible to solve for v as a function of V and t. Let's denote, for each $t \geq 0$, $\psi_t(v) = V$, so that we can write $v = \psi_t^{-1}(V)$, where

$$\psi_t^{-1}(V) \;=\; V\,e^{\lambda(t)} \;-\; E\int_0^t e^{\lambda(s)}\,ds. \tag{2.31}$$

For notational convenience, we write

$$\Lambda(t) \;=\; \int_0^t \big(1 - E\,\bar{\zeta}(s)\big)\,ds,$$

or, in other words $\Lambda(t) = t - \lambda(t)$.

Let $T > 0$ be fixed. The integral form of (2.29) in the time interval $[0,T]$ is

$$f^{\#}(v,t) \;=\; e^{-\Lambda(t)}\,f^{\#}(v,0) \;+\; e^{-\Lambda(t)}\int_0^t e^{\Lambda(\tau)}\,Q^{+}(f,f)^{\#}(v,\tau)\,d\tau, \quad \forall t \in [0,T]. \tag{2.32}$$

Using (2.31) we can rewrite (2.32) in terms of f

$$f(v,t) \;=\; \Gamma_{f_0}(f)(v,t), \tag{2.33}$$

where

$$\Gamma_{f_0}(f)(v,t) \;=\; e^{-\Lambda(t)}f_0\big(\psi_t^{-1}(v)\big) \;+\; e^{-\Lambda(t)}\int_0^t e^{\Lambda(\tau)}Q^{+}\big(f,f\big)\big(\psi_\tau\circ\psi_t^{-1}(v),\tau\big)\,d\tau. \tag{2.34}$$

Now we adapt the notion of mild solution to the setting at hand.

Definition 2.1. *A function f is said to be a mild solution to the initial value problem (2.25)–(2.27) on the time interval $[0,T]$ if $f(\cdot,t) \in L^1(\mathbb{R})$ and $f(\cdot,t)$ satisfies (2.33) for all $t \in [0,T]$.*

Theorem 2.3. *Let a non-negative f_0 with $\int_{\mathbb{R}} f_0(v)dv = 1$ be given. Then there exists a unique, non-negative $f \in C\big((0,\infty); L^1(\mathbb{R})\big)$ – mild solution to the initial value problem (2.25)-(2.27) and such that $\int_{\mathbb{R}} f(v,t)dv = 1$.*

Proof. Define a sequence of successive approximations $\{f^{(n)}(\cdot,t)\}_{n=1}^{\infty}$ inductively by setting

$$f^{(1)}(v,t) = 0, \tag{2.35}$$

$$f^{(n)}(v,t) = \Gamma_{f_0}\big(f^{(n-1)}\big)(v,t), \quad (n>1). \tag{2.36}$$

The monotonicity of Q^+ and the condition that f_0 is non-negative gives that the iterates are all non-negative.

It is also immediate that

$$f^{(2)}(v,t) \;=\; e^{-\Lambda(t)} f_0\big(\psi_t^{-1}(v)\big), \tag{2.37}$$

from which we see $f^{(2)}(v,t) \geq f^{(1)}(v,t)$ for all $v \in \mathbb{R}$. Suppose now, for some $n \geq 3$, that $f^{(n-1)} \geq f^{(n-2)}$ and consider the difference $f^{(n)} - f^{(n-1)}$, which is equal to

$$e^{-\Lambda(t)} \int_0^t e^{\Lambda(\tau)} \Big[Q^+\big(f^{(n-1)}, f^{(n-1)}\big) - Q^+\big(f^{(n-2)}, f^{(n-2)}\big) \Big] \big(\psi_\tau \circ \psi_t^{-1}(v), \tau\big)\, d\tau. \tag{2.38}$$

We recall, for any two functions f and g, that

$$Q^+(f,f) \;-\; Q^+(g,g) \;=\; Q^+(f-g,f) \;+\; Q^+(g,f-g).$$

This makes (2.38) to take the form

$$e^{-\Lambda(t)} \int_0^t e^{\Lambda(\tau)} \Big[Q^+\big(f^{(n-1)} - f^{(n-2)}, f^{(n-1)}\big) + Q^+\big(f^{(n-2)}, f^{(n-1)} - f^{(n-2)}\big) \Big]\, d\tau. \tag{2.39}$$

Since, by the induction hypothesis, $f^{(n-1)} - f^{(n-2)} \geq 0$ we use the monotonicity of Q^+ to conclude that the integral in (2.39) is non-negative. This shows, for each $t \geq 0$, and by induction for all n, that $f^{(n)}(v,t) \geq f^{(n-1)}(v,t)$ for all $v \in \mathbb{R}$.

Since $\int_{\mathbb{R}} f_0(v)dv = 1$ the result in (2.37) gives $\int_{\mathbb{R}} f^{(2)}(v,t)dv = e^{-t} \leq 1$. Suppose now, for some $n \geq 3$, that $\int_{\mathbb{R}} f^{(n-1)}(v,t)dv \leq 1$. Then

$$\int_{\mathbb{R}} f^{(n)}(v,t)dv \;=\; e^{-t} \;+\; e^{-t} \int_0^t e^{\tau} \int_{\mathbb{R}} Q^+\big(f^{(n-1)}, f^{(n-1)}\big)(z,\tau)dz\, d\tau.$$

We recall that

$$\int_{\mathbb{R}} Q^+\big(f^{(n-1)}, f^{(n-1)}\big)(z,\tau)dz \;=\; \int_{\mathbb{R}} f^{(n-1)}(z,\tau)dz \int_{\mathbb{R}} f^{(n-1)}(z_*,\tau)dz_*.$$

Writing $m^{(n)}(t) = \int_{\mathbb{R}} f^{(n)}(v,t)dv$, we find that

$$m^{(n)}(t) \;=\; e^{-t} \;+\; e^{-t} \int_0^t e^{\tau} m^{(n-1)}(\tau)^2 d\tau.$$

Using the induction hypothesis gives

$$m^{(n)}(t) \;=\; \int_{\mathbb{R}} f^{(n)}(v,t)\,dv \;\le\; e^{-t} \;+\; e^{-t}\int_0^t e^{\tau}d\tau \;=\; 1.$$

The bounded, monotonically increasing sequence $\{f^{(n)}(\cdot,t)\}_{n=1}^{\infty}$ of non-negative terms has a non-negative limit $f(\cdot,t)$ in $L^1(\mathbb{R})$ such that $f^{(n)} \to f$ as $n \to \infty$.

This limit satisfies (with the notation that $m(t) = \int_{\mathbb{R}} f(v,t)dv$)

$$m(t) \;=\; e^{-t} \;+\; e^{-t}\int_0^t e^{\tau} m(\tau)^2 d\tau.$$

The unique solution to this equation is $m(t) \equiv 1$. From this we conclude, by Levi's theorem that $\int_{\mathbb{R}} f(v,t)dv = 1$. This says that f solves (2.33), thereby showing that this f is a mild solution to (2.25)–(2.27). This completes the proof, apart from the uniqueness. That will follow from the calculations leading to the proof of Theorem 2.2. ■

Next we prove that f is a mild solution to (2.18), i.e. we prove Theorem 2.2. To do this it is enough to show that $\int_{\mathbb{R}} v\,f(v,t)\,dv = \bar{\zeta}(t)$. In general, to study the moments of f it is more convenient to study a different sequence $\{g^{(n)}(\cdot,t)\}_{n=1}^{\infty}$, which converges to f. This sequence is defined inductively by setting

$$g^{(1)}(v,t) \;= f_0(v), \tag{2.40}$$

$$g^{(n)}(v,t) \;= \Gamma_{f_0}\big(g^{(n-1)}\big)(v,t), \quad (n>1). \tag{2.41}$$

In the sequel we will also use the following equivalent form of (2.41):

$$e^{\Lambda(t)}\,g^{(n)}\big(\psi_t(v),t\big) \;=\; f_0(v) \;+\; \int_0^t e^{\Lambda(\tau)}\,Q^+\big(g^{(n-1)},g^{(n-1)}\big)\big(\psi_\tau(v),\tau\big)\,d\tau. \tag{2.42}$$

The sequence $\{g^{(n)}\}_{n=1}^{\infty}$ is defined in the same way as the sequence $\{f^{(n)}\}_{n=1}^{\infty}$ except that (2.35) is replaced by $g^{(1)} = f_0$. This sequence is not monotonous in general, but converges to f, as we shall demonstrate. The advantage of working with $\{g^{(n)}\}_{n=1}^{\infty}$ is that the first few moments can be computed explicitly and are independent of n.

Lemma 2.4. *Suppose that the non-negative f_0 is given, and that it satisfies*

$$\int_{\mathbb{R}} f_0(v)\,dv = 1, \;\; \int_{\mathbb{R}} v\,f_0(v)\,dv = \zeta_0, \;\; \textit{and} \;\; \int_{\mathbb{R}} v^2\,f_0(v)\,dv = 1.$$

Let

$$\bar{\zeta}(t) \;=\; \frac{\zeta_+ - \zeta_-\,C\,e^{-\sqrt{1+4E^2}\,t}}{1 - C\,e^{-\sqrt{1+4E^2}\,t}}.$$

Then, for each $t \geq 0$, and for each n

$$\int_{\mathbb{R}} g^{(n)}(v,t)\,dv \;=\; 1, \tag{2.43}$$

$$\int_{\mathbb{R}} v\, g^{(n)}(v,t)\,dv \;=\; \bar{\zeta}(t), \tag{2.44}$$

$$\int_{\mathbb{R}} v^2\, g^{(n)}(v,t)\,dv \;=\; 1. \tag{2.45}$$

Proof. By the assumption on f_0 we see that $\int_{\mathbb{R}} g^{(1)}(v,t)\,dv = 1$. We will prove by induction that the same holds for all n. Suppose now, for some $n \geq 2$, that $\int_{\mathbb{R}} g^{(n-1)}(v,t)\,dv = 1$. Integrating both sides of (2.42) over $\mathbb{R}$ with respect to v, and using the transformation (2.30) gives

$$e^t \int_{\mathbb{R}} g^{(n)}(v,t)dv \;=\; \int_{\mathbb{R}} f_0(v)dv \;+\; \int_0^t e^\tau \int_{\mathbb{R}} Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\,dv\,d\tau. \tag{2.46}$$

Note first that

$$\int_{\mathbb{R}} Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)dv \;=\; \left(\int_{\mathbb{R}} g^{(n-1)}(v,\tau)\,dv\right)^2, \tag{2.47}$$

which in turn is 1, by the induction hypothesis. Thus the right hand side of (2.46) equals

$$\int_{\mathbb{R}} f_0(v)\,dv \;+\; \int_0^t e^\tau\,d\tau,$$

which sums up to be e^t. Thus we conclude, for all $t \geq 0$, and by induction for all n, that

$$\int_{\mathbb{R}} g^{(n)}(v,t)\,dv \;=\; 1.$$

To prove (2.44), we multiply both sides of (2.41) by v, and integrate the result over $\mathbb{R}$ with respect to v to get

$$\begin{aligned}\int_{\mathbb{R}} v\, g^{(n)}(v,t)dv = e^{-\Lambda(t)} \int_{\mathbb{R}} v f_0\big(\psi_t^{-1}(v)\big)dv \;+\\ + e^{-\Lambda(t)} \int_{\mathbb{R}} \int_0^t e^{\Lambda(\tau)} v Q^+\big(g^{(n-1)}, g^{(n-1)}\big)\,\big(\psi_\tau \circ \psi_t^{-1}(v), \tau\big)\,d\tau dv.\end{aligned} \tag{2.48}$$

Use of the transformation (2.31) makes the first term in the sum (2.48) to be

$$\begin{aligned} e^{-\Lambda(t)} \int_{\mathbb{R}} v\, f_0\big(\psi_t^{-1}(v)\big)dv \;&=\; e^{-t+\lambda(t)} \int_{\mathbb{R}} e^{-\lambda(t)}\big(v + E\,q(0,t)\big) f_0(v) e^{-\lambda(t)} dv \\ &=\; e^{-t-\lambda(t)} \left(\int_{\mathbb{R}} v\, f_0(v)\,dv + E\,q(0,t) \int_{\mathbb{R}} f_0(v)\,dv\right) \\ &=\; e^{-t-\lambda(t)}\big(\zeta_0 + E\,q(0,t)\big), \end{aligned} \tag{2.49}$$

where $q(\tau,t) = \int_\tau^t e^{\lambda(s)} ds$.

Using (2.30) and (2.31) once more, the second term in the sum (2.48) equals

$$e^{-t-\lambda(t)} \int_{\mathbb{R}} \int_0^t e^\tau \Big(v\, e^{\lambda(\tau)} + E\, q(\tau,t) \Big)\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, d\tau\, dv.$$

This in turn is

$$\begin{aligned} & e^{-t-\lambda(t)} \int_0^t e^{\tau+\lambda(\tau)} \int_{\mathbb{R}} v\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv\, d\tau \; + \\ & \quad + \; e^{-t-\lambda(t)} E \int_0^t e^\tau\, q(\tau,t) \int_{\mathbb{R}} Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv\, d\tau. \end{aligned} \tag{2.50}$$

Now we use the result $\int_{\mathbb{R}} v\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv = 0$ with (2.43) and (2.47) so that the sum in (2.50) reduces to

$$E\, e^{-t-\lambda(t)} \int_0^t e^\tau\, q(\tau,t)\, d\tau. \tag{2.51}$$

Combining (2.49) and (2.51) makes (2.48) to take the form

$$\int_{\mathbb{R}} v\, g^{(n)}(v,t)\, dv \;=\; e^{-t-\lambda(t)} \left(\zeta_0 \;+\; E\, q(0,t) \;+\; E \int_0^t e^\tau\, q(\tau,t)\, d\tau \right).$$

We further note, through integration by parts, that

$$\int_0^t e^\tau\, q(\tau,t)\, d\tau \;=\; -q(0,t) \;+\; \int_0^t e^{s+\lambda(s)}\, ds.$$

Thus we have

$$\int_{\mathbb{R}} v\, g^{(n)}(v,t)\, dv \;=\; \zeta_0\, e^{-t-\lambda(t)} \;+\; E\, e^{-t-\lambda(t)} \int_0^t e^{s+\lambda(s)}\, ds. \tag{2.52}$$

We are now left to show that the right hand side of (2.52) and $\bar\zeta(t)$ are equal. Towards this, we denote the right hand side of (2.52) by $\hat\zeta(t)$, namely let

$$\hat\zeta(t) \;=\; \zeta_0\, e^{-t-\lambda(t)} \;+\; E\, e^{-t-\lambda(t)} \int_0^t e^{s+\lambda(s)}\, ds.$$

Now we see that, $\hat\zeta(t)$ fulfills

$$\frac{d}{dt}\Big(e^t\, \hat\zeta(t) \Big) \;=\; E\, e^t \Big(1 - \bar\zeta(t)\, \hat\zeta(t) \Big),$$

with $\hat\zeta(0) = \zeta_0$. Similarly, $\bar\zeta(t)$ satisfies

$$\frac{d}{dt}\Big(e^t\, \bar\zeta(t) \Big) \;=\; E\, e^t \Big(1 - \bar\zeta(t)\, \bar\zeta(t) \Big),$$

with $\bar{\zeta}(0) = \zeta_0$.

Since $\bar{\zeta}(t)$ is bounded we conclude that $\hat{\zeta}(t) = \bar{\zeta}(t)$. This together with (2.52) finally implies the desired result that

$$\int_{\mathbb{R}} v\, g^{(n)}(v,t)\, dv \;=\; \bar{\zeta}(t).$$

To prove (2.45) we first multiply both sides of (2.42) by v^2 and integrate over $\mathbb{R}$ with respect to v, to get

$$\begin{aligned} e^{\Lambda(t)} \int_{\mathbb{R}} v^2 g^{(n)}\big(\psi_t(v),t\big)dv = \int_{\mathbb{R}} v^2\, f_0(v)dv \\ + \int_{\mathbb{R}}\int_0^t e^{\Lambda(\tau)} v^2 Q^+\big(g^{(n-1)}, g^{(n-1)}\big)\big(\psi_\tau(v),\tau\big)d\tau dv. \end{aligned} \tag{2.53}$$

With the transformation (2.30) the left hand side of (2.53) can be rewritten as

$$e^t \int_{\mathbb{R}} \Big(v^2 e^{2\lambda(t)} - 2Eq(0,t)e^{\lambda(t)}v + E^2 q(0,t)^2\Big) g^{(n)}(v,t)dv,$$

which in turn equals

$$e^{t+2\lambda(t)} \int_{\mathbb{R}} v^2 g^{(n)}(v,t)dv - 2Eq(0,t)e^{t+\lambda(t)} \int_{\mathbb{R}} v g^{(n)}(v,t)dv + E^2 q(0,t)^2 e^t \int_{\mathbb{R}} g^{(n)}(v,t)dv.$$

Using the results from (2.43) and (2.44) we thus write

$$e^{\Lambda(t)} \int_{\mathbb{R}} v^2\, g^{(n)}\big(\psi_t(v),t\big)\, dv \;=\; e^{t+2\lambda(t)}\, M_2^{(n)}(t) - 2\, E\, \bar{\zeta}(t)\, q(0,t)\, e^{t+\lambda(t)} + E^2\, q(0,t)^2\, e^t,$$

where $M_2^{(n)}(t) = \int_{\mathbb{R}} v^2 g^{(n)}(v,t)dv$.

Use of (2.30) and (2.31) makes the second term in the sum at the right hand side of (2.53) to take the form

$$\int_0^t e^\tau \int_{\mathbb{R}} \Big(v^2\, e^{2\lambda(\tau)} - 2\, E\, q(\tau)\, e^{\lambda(\tau)}\, v + E^2\, q(\tau)^2\Big) Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)dvd\tau.$$

This can be split into three terms as

$$\begin{aligned} \int_0^t e^{\tau+2\lambda(\tau)} \int_{\mathbb{R}} v^2\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv\, d\tau \\ - 2\, E \int_0^t q(\tau)\, e^{\tau+\lambda(\tau)} \int_{\mathbb{R}} v\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv\, d\tau \\ + \; E^2 \int_0^t e^\tau\, q(\tau)^2 \int_{\mathbb{R}} Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\, dv\, d\tau. \end{aligned} \tag{2.54}$$

We recall that

$$\begin{aligned}
\int_{\mathbb{R}} Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\,dv \;&=\; 1,\\
\int_{\mathbb{R}} v\,Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\,dv \;&=\; 0,\ \text{and}\\
\int_{\mathbb{R}} v^2\,Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)\,dv \;&=\; \int_{\mathbb{R}} v^2\,g^{(n-1)}(v,\tau)\,dv,
\end{aligned} \tag{2.55}$$

so that the sum in (2.54) reduces to

$$\int_0^t e^{\tau+2\lambda(\tau)}\,M_2^{(n-1)}(\tau)\,d\tau \;+\; E^2\int_0^t e^{\tau}\,q(\tau)^2\,d\tau.$$

Now we put the pieces together and rearrange the terms so as to rewrite (2.53) as

$$\begin{aligned}
e^{t+2\lambda(t)}M_2^{(n)}(t) \;&=2E\bar{\zeta}(t)q(0,t)e^{t+\lambda(t)} \;-\; E^2q(0,t)^2e^t \;+1\\
&\quad+\;\int_0^t e^{\tau+2\lambda(\tau)}M_2^{(n-1)}(\tau)d\tau \;+\; E^2\int_0^t e^{\tau}\,q(\tau)^2d\tau.
\end{aligned} \tag{2.56}$$

The next step is to differentiate (2.56) with respect to time, but first we note that

$$\begin{aligned}
2\,E\,\frac{d}{dt}\Big(\bar{\zeta}(t)\,q(0,t)\,e^{t+\lambda(t)}\Big) \;&=2\,\lambda''(t)q(0,t)e^{t+\lambda(t)} \;+\; 2\big(\lambda'(t)\\
&\quad+\;\lambda'(t)^2\big)q(0,t)\,e^{t+\lambda(t)} \;+\; 2\,\lambda'(t)e^{t+2\lambda(t)}.
\end{aligned}$$

We also have $\lambda''(t) = E^2 - \lambda'(t) - \lambda'(t)^2$, so that

$$2E\frac{d}{dt}\Big(\bar{\zeta}(t)\,q(0,t)\,e^{t+\lambda(t)}\Big) \;=\; 2E^2q(0,t)e^{t+\lambda(t)} \;+\; 2\lambda'(t)e^{t+2\lambda(t)}.$$

Since $\frac{d}{dt}q(0,t) = e^{\lambda(t)}$,

$$-E^2\frac{d}{dt}\left(q(0,t)^2\,e^t\right) \;=\; -2E^2q(0,t)e^{t+\lambda(t)} \;-\; E^2q(0,t)^2e^t.$$

Computing the time derivatives of the last two terms on the right hand side of (2.56) we have $e^{t+2\lambda(t)}\,M_2^{(n-1)}(t)$ and $E^2\,e^t\,q(0,t)^2$ respectively.

Combining all these terms gives

$$\frac{d}{dt}\Big(e^{t+2\lambda(t)}M_2^{(n)}(t)\Big) \;=\; 2\lambda'(t)e^{t+2\lambda(t)} \;+\; e^{t+2\lambda(t)}M_2^{(n-1)}(t).$$

We rewrite the right hand side of this and get

$$\frac{d}{dt}\Big(e^{t+2\lambda(t)}\,M_2^{(n)}(t)\Big) \;=\; 2\,\lambda'(t)\,e^{t+2\lambda(t)} \;+\; e^{t+2\lambda(t)} \;+\; e^{t+2\lambda(t)}\Big(M_2^{(n-1)}(t) - 1\Big).$$

Supposing that $M_2^{(n-1)}(t) = 1$, then the last term in the above sum is zero so that the remaining terms can be rewritten as

$$\frac{d}{dt}\left(e^{t+2\lambda(t)}\, M_2^{(n)}(t)\right) \;=\; \frac{d}{dt}\left(e^{t+2\lambda(t)}\right).$$

Integration and rearrangement of the terms gives

$$M_2^{(n)}(t) \;=\; \left(M_2^{(n)}(0) - 1\right) e^{-t-2\lambda(t)} \;+\; 1.$$

This leads to the result that $M_2^{(n)}(t) = 1$, namely

$$\int_{\mathbb{R}} v^2\, g^{(n)}(v,t)\, dv \;=\; 1.$$

This completes the proof of Lemma 2.4. ■

Proof of Theorem 2.2: It suffices to prove $g^{(n)} \to f$ in L^1, because in view of the boundedness of $\int_{\mathbb{R}} v^2 g^{(n)} dv$ this would imply that $\int_{\mathbb{R}} v f(v,t)\, dv = \bar{\zeta}$.

By construction $f^n \le g^n$. We thus have

$$\int_{\mathbb{R}} \left|f - g^{(n)}\right| dv \;=\; 2\int_{\{f \ge g^{(n)}\}} \left(f - g^{(n)}\right) dv \;-\; \int_{\mathbb{R}} \left(f - g^{(n)}\right) dv.$$

But $\int_{\mathbb{R}} f(v,t) dv = \int_{\mathbb{R}} g^{(n)}(v,t) dv = 1$, so we find

$$\begin{aligned}\int_{\mathbb{R}} \left|f - g^{(n)}\right| dv \;&= 2\int_{\{f \ge g^{(n)}\}} \left(f - g^{(n)}\right) dv \\ &\le 2\int_{\mathbb{R}} \left(f - f^{(n)}\right) dv \;\to\; 0,\end{aligned}$$

when $n \to \infty$. In the following section we will prove that $\int_{\mathbb{R}} v^4 g^{(n)} dv$ is uniformly bounded in n, and from that we may conclude also that $\int_{\mathbb{R}} v^2 f(v,t)\, dv = 1$.

Almost the same argument implies the uniqueness result in Theorem 2.3. In fact, if $f_*(v,t)$ is any solution to (2.33) then

$$f_*(v,t) \;=\; \Gamma_{f_0}(f_*)(v,t).$$

The monotonicity of Q^+, and thus that of Γ_{f_0}, then implies that, for all n,

$$f^{(n)}(v,t) \;\le\; f_*(v,t),$$

and the same holds for $f(v,t) \;=\; \lim_{n\to\infty} f^{(n)}(v,t)$. But

$$\int_{\mathbb{R}} f_*(v,t) dv \;=\; \int_{\mathbb{R}} f(v,t) dv \;=\; 1,$$

and thus $f_* = f$. ■

2.4 On higher order moments

What we have studied in Lemma 2.4 is an explicit form of the first few moments of the iterates. In this section we continue to look at the third and fourth moments of the iterates in detail, thereby demonstrating how the method can be used to get a general form for all other higher order moments of the iterates. In a similar way, we derive a general form to the higher order moments of the solution directly from the main equation.

Notation. For $k = 1, 2, \ldots$, let $M_k^{(n)}(t)$ denote moment of order k of the iterate $g^{(n)}(v,t)$, and let $M_k(t)$ denote moment of order k of the solution $f(v,t)$, i.e.

$$\begin{aligned} M_k^{(n)}(t) &= \int_{\mathbb{R}} v^k \, g^{(n)}(v,t)\, dv, \\ M_k(t) &= \int_{\mathbb{R}} v^k \, f(v,t)\, dv. \end{aligned}$$

We start with the third moment of the iterates. We multiply both sides of (2.42) by v^3 and integrate both sides of the resulting expression over $\mathbb{R}$ with respect to v to get

$$\begin{aligned} e^{\Lambda(t)} \int_{\mathbb{R}} v^3 g^{(n)}\big(\psi_t(v),t\big) dv = \int_{\mathbb{R}} v^3 f_0(v) dv \\ + \int_{\mathbb{R}} \int_0^t e^{\Lambda(\tau)}\, v^3\, Q^+\big(g^{(n-1)}, g^{(n-1)}\big)\big(\psi_\tau(v),\tau\big) d\tau dv. \end{aligned} \tag{2.57}$$

Use of the transformation (2.30) turns the left hand side of (2.57) in to

$$e^t \int_{\mathbb{R}} \Big(v^3 e^{3\lambda(t)} \; - \; 3\,E\,q(t)\, e^{2\lambda(t)}\, v^2 \; + \; 3\,E^2\, q(t)^2\, e^{\lambda(t)}\, v \; - \; E^3\, q(t)^3 \Big)\, g^{(n)}(v,t)\, dv,$$

where $q(t) = q(0,t)$. This in turn equals

$$\begin{aligned} e^{t+3\lambda(t)} \int_{\mathbb{R}} v^3 g^{(n)}(v,t)\, dv \; - \; 3\,E\,q(t)\, e^{t+2\lambda(t)} \int_{\mathbb{R}} v^2 g^{(n)}(v,t) dv \\ + \, 3\,E^2\, q(t)^2 e^{t+\lambda(t)} \int_{\mathbb{R}} v g^{(n)}(v,t) dv - \; E^3\, q(t)^3\, e^t \int_{\mathbb{R}} g^{(n)}(v,t) dv. \end{aligned} \tag{2.58}$$

By Lemma 2.4, (2.58) equals

$$e^{t+3\lambda(t)} M_3^{(n)}(t) \; - \; 3\,E\,q(t)\, e^{t+2\lambda(t)} \; + \; 3\,E^2\, q(t)^2\, e^{t+\lambda(t)} \bar{\zeta}(t) \; - \; E^3\, q(t)^3\, e^t. \tag{2.59}$$

Using (2.30), the second term in the sum on the right hand side of (2.57) takes the form

$$\begin{aligned} \int_0^t e^{\tau+3\lambda(\tau)} \int_{\mathbb{R}} v^3 Q^+ dv\, d\tau \; - \; 3E \int_0^t q(\tau)\, e^{\tau+2\lambda(\tau)} \int_{\mathbb{R}} v^2 Q^+ dv\, d\tau \; + \\ + \; 3E^2 \int_0^t q(\tau)^2 e^{\tau+\lambda(\tau)} \int_{\mathbb{R}} v Q^+ dv d\tau \; - \; E^3 \int_0^t q(\tau)^3 e^\tau \int_{\mathbb{R}} Q^+ dv d\tau, \end{aligned} \tag{2.60}$$

where $Q^+ = Q^+\big(g^{(n-1)}, g^{(n-1)}\big)(v,\tau)$. Noting that $\int_{\mathbb{R}} v^3 Q^+ dv = 0$ and using (2.55) the sum (2.60) reduces to

$$-3\,E\int_0^t q(\tau)\,e^{\tau+2\lambda(\tau)}\,d\tau \;-\; E^3\int_0^t q(\tau)^3\,e^{\tau}\,d\tau. \tag{2.61}$$

We use (2.59) and (2.61) in (2.57), rearrange the terms so that

$$\begin{aligned} e^{t+3\lambda(t)}M_3^{(n)}(t) \;&= M_3^{(n)}(0) \;+\; 3Eq(t)e^{t+2\lambda(t)} \;-\; 3E^2q(t)^2e^{t+\lambda(t)}\bar{\zeta}(t) \;+ \\ &+\; E^3q(t)^3e^t \;-\; 3E\int_0^t q(\tau)e^{\tau+2\lambda(\tau)}d\tau \;-\; E^3\int_0^t q(\tau)^3e^{\tau}d\tau. \end{aligned}$$

Taking the time derivative of both sides we have

$$\begin{aligned} \frac{d}{dt}\Big(e^{t+3\lambda(t)}M_3^{(n)}(t)\Big) \;&= 3Ee^{t+3\lambda(t)} + 3Eq(t)e^{t+2\lambda(t)} + 6E\lambda'(t)q(t)e^{t+2\lambda(t)} \\ &-\; 6E\lambda'(t)q(t)e^{t+2\lambda(t)} - 3E^3q(t)^2e^{t+\lambda(t)} + 3E^3q(t)^2e^{t+\lambda(t)} \\ &+\; E^3q(t)^3e^t - 3Eq(t)e^{t+2\lambda(t)} - E^3q(t)^3e^t, \end{aligned}$$

which, after simplification, reduces to

$$\frac{d}{dt}\Big(e^{t+3\lambda(t)}M_3^{(n)}(t)\Big) \;=\; 3\,E\,e^{t+3\lambda(t)}. \tag{2.62}$$

Integration gives

$$M_3^{(n)}(t) \;=\; M_3^{(n)}(0)\,e^{-t-3\lambda(t)} \;+\; 3E\,e^{-t-3\lambda(t)}\int_0^t e^{s+3\lambda(s)}ds.$$

Since this is independent of n we have, as $n\to\infty$, $M_3^{(n)}(t)\to M_3(t)$ where

$$M_3(t) \;=\; M_3(0)\,e^{-t-3\lambda(t)} \;+\; 3\,E\,e^{-t-3\lambda(t)}\int_0^t e^{s+3\lambda(s)}ds.$$

To study the fourth moment of the iterates we multiply both sides of (2.42) by v^4 and integrate both sides of the resulting expression over $\mathbb{R}$ with respect to v. This gives

$$\begin{aligned} e^{\Lambda(t)}\int_{\mathbb{R}} v^4 g^{(n)}\big(\psi_t(v),t\big)dv = &\int_{\mathbb{R}} v^4 f_0(v)dv \;+ \\ &+\; \int_{\mathbb{R}}\int_0^t e^{\Lambda(\tau)}v^4Q^+\big(g^{(n-1)},g^{(n-1)}\big)\big(\psi_\tau(v),\tau\big)d\tau dv. \end{aligned} \tag{2.63}$$

We rewrite this expression using (2.30), and obtain

$$e^{\Lambda(t)}\int_{\mathbb{R}} v^4 g^{(n)}\big(\psi_t(v),t\big)dv \;=\; \sum_{j=0}^{4}(-1)^{4-j}\binom{4}{j}\big(E\,q(t)\big)^{4-j}e^{t+j\lambda(t)}M_j^{(n)}(t), \tag{2.64}$$

which in turn equals

$$\sum_{j=0}^{2}\binom{4}{j}\big(-E\,q(t)\big)^{4-j}e^{t+j\lambda(t)}M_j^{(n)}(t)-4Eq(t)e^{t+3\lambda(t)}M_3^{(n)}(t)+e^{t+4\lambda(t)}M_4^{(n)}(t). \quad (2.65)$$

Another use of (2.30) makes the second term in the sum at the right hand side of (2.63) to be

$$\sum_{j=0}^{3}\binom{4}{j}(-E)^{4-j}\int_0^t q(\tau)^{4-j}e^{\tau+j\lambda(\tau)}\int_{\mathbb{R}}v^j\,Q^+dvd\tau\;+\;\int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}}v^4\,Q^+dvd\tau,$$

where again $Q^+=Q^+\big(g^{(n-1)},g^{(n-1)}\big)(v,\tau)$.

Collecting and rearranging the terms gives

$$\begin{aligned}e^{t+4\lambda(t)}M_4^{(n)}(t)\;&=M_4^{(n)}(0)+4Eq(t)e^{t+3\lambda(t)}M_3^{(n)}(t)+\int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}}v^4\,Q^+dvd\tau\\&+\sum_{j=0}^{2}(-1)^{j+1}\binom{4}{j}\big(E\,q(t)\big)^{4-j}e^{t+j\lambda(t)}M_j^{(n)}(t)\\&+\sum_{j=0}^{1}\binom{4}{2j}E^{4-2j}\int_0^t q(\tau)^{4-2j}e^{\tau+2j\lambda(\tau)}M_0^{(n-1)}(\tau)M_j^{(n-1)}(\tau)d\tau.\end{aligned} \quad (2.66)$$

Here we have used

$$\begin{aligned}\int_{\mathbb{R}}Q^+\big(g^{(n-1)},g^{(n-1)}\big)(v,\tau)dv\;&=\;M_0^{(n-1)}(\tau)M_0^{(n-1)}(\tau),\\\int_{\mathbb{R}}v^2\,Q^+\big(g^{(n-1)},g^{(n-1)}\big)(v,\tau)dv\;&=\;M_0^{(n-1)}(\tau)M_2^{(n-1)}(\tau).\end{aligned}$$

Of the terms in the right hand side of (2.66) the only one depending on n is

$$\int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}}v^4\,Q^+\big(g^{(n-1)},g^{(n-1)}\big)(v,\tau)\,dv.$$

Therefore

$$\begin{aligned}&e^{t+4\lambda(t)}\Big(M_4^{(n)}(t)-M_4^{(n-1)}(t)\Big)\\&=\;\int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}}v^4\Big(Q^+\big(g^{(n-1)},g^{(n-1)}\big)-Q^+\big(g^{(n-2)},g^{(n-2)}\big)\Big)\,dvd\tau\end{aligned}$$

which in turn equals

$$\begin{aligned}\int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}^2}\int_{-\pi}^{\pi}&\Big[g^{(n-1)}(v)g^{(n-1)}(v_*)-g^{(n-2)}(v)g^{(n-2)}(v_*)\Big]\\&\times\;\big[v\cos\theta-v_*\sin\theta\big]^4\frac{1}{2\pi}\,d\theta\,dv\,dv_*\,d\tau.\end{aligned} \quad (2.67)$$

Here we use

$$\begin{aligned} & g^{(n-1)}(v)g^{(n-1)}(v_*) \;-\; g^{(n-2)}(v)g^{(n-2)}(v_*) \\ &\quad = \;\Big(g^{(n-1)}(v) - g^{(n-2)}(v)\Big)\, g^{(n-1)}(v_*) \;+\; g^{(n-2)}(v)\,\Big(g^{(n-1)}(v_*) - g^{(n-2)}(v_*)\Big)\,, \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{2\pi}\int_{-\pi}^{\pi} \big(v\cos\theta - v_*\sin\theta\big)^4 d\theta \\ &\quad = \;\; v^4\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos^4\theta\, d\theta \;+\; 6v^2v_*^2\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos^2\theta\sin^2\theta\, d\theta \;+\; v_*^4\frac{1}{2\pi}\int_{-\pi}^{\pi}\sin^4\theta\, d\theta. \\ &\quad = \;\; \frac{3}{8}v^4 \;+\; \frac{3}{4}v^2v_*^2 \;+\; \frac{3}{8}v_*^4. \end{aligned}$$

Therefore (2.67) is equal to

$$\begin{aligned} & \int_0^t e^{\tau+4\lambda(\tau)}\int_{\mathbb{R}^2}\Big[\,\Big(g^{(n-1)}(v) - g^{(n-2)}(v)\Big)\, g^{(n-1)}(v_*) \;+ \\ & \quad +\; g^{(n-2)}(v)\,\Big(g^{(n-1)}(v_*) - g^{(n-2)}(v_*)\Big)\Big]\,\Big(\frac{3}{8}v^4 \;+\; \frac{3}{4}v^2v_*^2 \;+\; \frac{3}{8}v_*^4\Big)\, dv\, dv_*\, d\tau. \end{aligned} \tag{2.68}$$

Note that

$$\int_{\mathbb{R}} v^2\,\Big(g^{(n-1)}(v) - g^{(n-2)}(v)\Big)\, dv \;=\; 0,$$

and recall also that $\int_{\mathbb{R}} g^{(n)}(v)dv = 1$. What remains after simplification is

$$\frac{3}{4}\int_0^t e^{\tau+4\lambda(\tau)}\,\Big(M_4^{(n-1)}(\tau) - M_4^{(n-2)}(\tau)\Big)\, d\tau.$$

So we have

$$M_4^{(n)}(t) - M_4^{(n-1)}(t) \;=\; \frac{3}{4}\,e^{-t-4\lambda(t)}\int_0^t e^{\tau+4\lambda(\tau)}\,\Big(M_4^{(n-1)}(\tau) - M_4^{(n-2)}(\tau)\Big)\, d\tau.$$

It then follows that $\{M_4^{(n)}\}_{n=1}^{\infty}$ is convergent in a sufficiently small interval $0 < t < \bar{t}$ and that the limit $M_4(t)$ must satisfy

$$\frac{d}{dt}M_4(t) \;=\; -4E\zeta(t)M_4(t) + 4EM_3(t) - M_4(t) + \frac{3}{4}M_4(t) + \frac{3}{4}. \tag{2.69}$$

The solution can be extended from the interval $(0, \bar{t}\,]$ to the whole of $\mathbb{R}^+$, and we conclude from (2.69) that $M_4(t)$ remains bounded for all t if it is bounded at $t = 0$.

The third moment, $M_3(t)$ satisfies the equation

$$\frac{d}{dt}M_3(t) \;=\; 3E \;-\; 3E\zeta(t)M_3(t) \;-\; M_3(t).$$

By formal calculations we can derive an explicit differential equation for any moment $M_k(t)$, where k is a positive integer. We recall the main equation

$$\frac{\partial f}{\partial t} \; + \; E\,\frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\,v\big)f\Big) \;=\; Q(f,f). \tag{2.70}$$

Write $Q = Q^+ - f$, multiply both sides of (2.70) by v^k, and integrate with respect to v, to get

$$\int_{\mathbb{R}} v^k \frac{\partial f}{\partial t} dv + E\int_{\mathbb{R}} v^k \frac{\partial}{\partial v}\Big(\big(1-\zeta(t)\,v\big)f\Big)dv = \int_{\mathbb{R}} v^k Q^+(f,f)(v)dv - \int_{\mathbb{R}} v^k f(v,t)dv. \tag{2.71}$$

With integration by parts and rearrangement of the terms, (2.71) can be rewritten as

$$\frac{d}{dt}M_k(t) \;=\; k\,E\,M_{k-1}(t) \;-\; k\,E\,\zeta(t)\,M_k(t) \;-\; M_k(t) \;+\; \int_{\mathbb{R}} v^k\,Q^+(f,f)(v)\,dv. \tag{2.72}$$

The last term in the sum (2.72), which involves the integral of Q^+ can always be calculated in terms of $M_j(t)$ where $j \le k$. For this we first note, for each odd k

$$\int_{\mathbb{R}} v^k Q^+(f,f)(v)dv \;=\; \int_{\mathbb{R}^2}\int_{-\pi}^{\pi} (v')^k f(v) f(v_*)\frac{1}{2\pi}d\theta dv_* dv \;=\; 0.$$

Thus, for each odd k, (2.72) takes the form

$$\frac{d}{dt}M_k(t) \;=\; k\,E\,M_{k-1}(t) \;-\; k\,E\,\zeta(t)\,M_k(t) \;-\; M_k(t). \tag{2.73}$$

If k is even, so that $k = 2m$ for some $m \in \mathbb{N}$, we have that

$$\begin{aligned}\int_{\mathbb{R}} v^k\,Q^+(f,f)(v)\,dv \;&=\; \int_{\mathbb{R}} v^{2m}\,Q^+(f,f)(v)\,dv \\ &=\; \int_{\mathbb{R}}\int_{\mathbb{R}}\int_{-\pi}^{\pi} (v')^{2m} f(v)\,f(v_*)\frac{1}{2\pi}d\theta\,dv_*\,dv.\end{aligned}$$

This in turn equals

$$\begin{aligned}&\sum_{j=0}^{2m}\binom{2m}{j}\int_{\mathbb{R}} v^{2m-j}\,f\,dv\int_{\mathbb{R}} v^j\,f\,dv\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos^{2m-j}\theta\,\sin^j\theta\,d\theta\right] \\ &\qquad=\; \sum_{j=0}^{m}\binom{2m}{2j}\frac{(2j-1)!!\,(2m-2j-1)!!}{(2m)!!}\int_{\mathbb{R}} v^{2m-2j}f\,dv\int_{\mathbb{R}} v^{2j}f\,dv.\end{aligned}$$

We thus have, for each even k

$$\int_{\mathbb{R}} v^k Q^+(f,f)(v)dv \;=\; \sum_{j=0}^{k/2}\binom{k}{2j}\frac{(2j-1)!!\,(k-2j-1)!!}{k!!}M_{k-2j}(t)M_{2j}(t). \tag{2.74}$$

The double factorial $m!!$ is defined by

$$m!! = \begin{cases} m \cdot (m-2) \cdot \ldots 5 \cdot 3 \cdot 1, & m > 0 \quad \text{odd} \\ m \cdot (m-2) \cdot \ldots 6 \cdot 4 \cdot 2, & m > 0 \quad \text{even} \\ 1, & m = -1,\ 0. \end{cases}$$

We thus have established the result that

Lemma 2.5. *For $k = 1, 2, \ldots$, let $M_k(t)$ denote moment of order k of the solution $f(v,t)$ to (2.25). Then $M_k(t)$ satisfies the differential equation*

$$\frac{d}{dt} M_k(t) \ = \ k\, E\, M_{k-1}(t) \ - \ k\, E\, \zeta(t)\, M_k(t) \ - \ M_k(t) \ + \ \int_{\mathbb{R}} v^k Q^+(f,f)(v) dv, \quad (2.75)$$

where the integral in the last term can be computed in terms of $M_j(t)$, $j \leq k$.

To illustrate how higher order moments of the solution evolve in time we take a closer look at the first few cases of (2.72). Towards this, we notice that

$$\begin{aligned} \int_{\mathbb{R}} v^2\, Q^+(f,f)(v)\, dv \ &= \ M_2(t), \\ \int_{\mathbb{R}} v^4\, Q^+(f,f)(v)\, dv \ &= \ \frac{3}{4} M_4(t) \ + \ \frac{3}{4} M_2(t) M_2(t), \\ \int_{\mathbb{R}} v^6\, Q^+(f,f)(v)\, dv \ &= \ \frac{5}{8} M_6(t) \ + \ \frac{15}{8} M_4(t) M_2(t). \end{aligned}$$

These results used in (2.72) give

$$\begin{aligned} \frac{d}{dt} M_2(t) \ &= \ 2\, E\, \zeta(t) \ - \ 2\, E\, \zeta(t)\, M_2(t), \\ \frac{d}{dt} M_4(t) \ &= \ 4\, E\, M_3(t) \ - \ 4\, E\, \zeta(t)\, M_4(t) \ - \ \frac{1}{4} M_4(t) \ + \ \frac{3}{4} M_2(t) M_2(t), \\ \frac{d}{dt} M_6(t) \ &= \ 6\, E\, M_5(t) \ - \ 6\, E\, \zeta(t)\, M_6(t) \ - \ \frac{3}{8} M_6(t) \ + \ \frac{15}{8} M_4(t) M_2(t). \end{aligned}$$

We then solve the resulting system of differential equations, where $k = 1, 2, \ldots, 7$, with initial data $M_k(0) = 0$ for $k = 1, 3, 5, 7$; $M_2(0) = 1$, $M_4(0) = 3$, and $M_6(0) = 15$. Figure 2.2 shows part of this result, illustrating the evolution of the first four moments of the solution f. The evolution of the other moments, namely $M_k(t)$ with $k = 5, 6, 7$, are shown in Figure 2.3. Here we use $E = \sqrt{2}$. This choice of E and $M_k(0)$ will enable us to compare these results with those obtained from Monte Carlo simulations which are presented in Figure 4.10 in the section on numerical results.

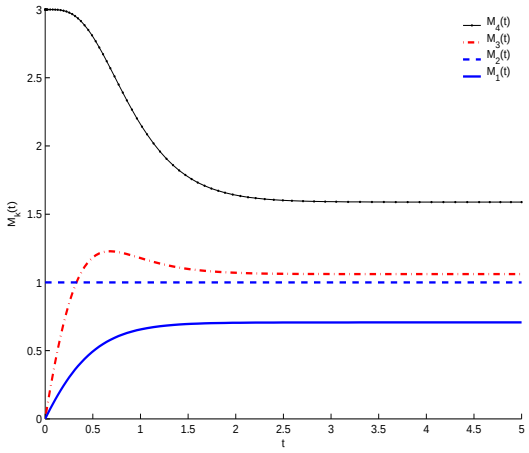

Figure 2.2: The evolution of moments of the solution, $M_k(t)$ with $k = 1, 2, 3, 4$, according to (2.72), ($E = \sqrt{2}$).

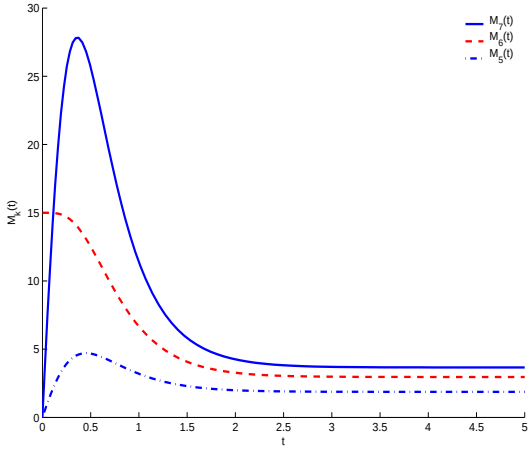

Figure 2.3: The evolution of moments of the solution, $M_k(t)$ with $k = 5, 6, 7$, according to (2.72), ($E = \sqrt{2}$).

2.5 The stationary problem

In this section we formulate the stationary problem associated with the time-dependent thermostatted Kac equation (2.8) and present a summary of the main results in Paper I. As an extension of these results, we also discuss the singular behavior that $Q^+(f,f)$ shows at those points where the stationary solution f has singularities.

A time-independent solution of the thermostatted Kac equation satisfies the following equation

$$E\,\frac{d}{dv}\Big(\big(1-\zeta\,v\big)\,f(v)\Big) \;=\; Q(f,f)(v), \tag{2.76}$$

where

$$\zeta \;=\; \int_{\mathbb{R}} v\,f(v)\,dv, \tag{2.77}$$

and

$$Q(f,f)(v) \;=\; \int_{\mathbb{R}}\int_{-\pi}^{\pi}\Big(f(v')\,f(v'_*)-f(v)\,f(v_*)\Big)\,\frac{1}{2\pi}\,d\theta\,dv_*. \tag{2.78}$$

With the condition $\int_{\mathbb{R}} f(v)\,dv=1$, the collision integral (2.78) can be rewritten as

$$Q(f,f)(v) \;=\; Q^+(f,f)(v)-f(v). \tag{2.79}$$

Now we multiply both sides of (2.76) by v, integrate the resulting expression with respect to v, and note that $\int_{\mathbb{R}} vQ^+(f,f)(v)dv \;=\; \int_{\mathbb{R}} v'Q^+(f,f)(v)dv \;=\; 0$. This gives, on the one hand

$$\int_{\mathbb{R}} v\,Q(f,f)(v)\,dv \;=\; \int_{\mathbb{R}} v\,Q^+(f,f)(v)\,dv-\int_{\mathbb{R}} v\,f(v)\,dv \;=\; -\zeta,$$

and on the other hand, by partial integration,

$$\int_{\mathbb{R}} v\frac{d}{dv}\Big(\big(1-\zeta\,v\big)f(v)\Big)dv \;=\; -\int_{\mathbb{R}}\big(1-\zeta\,v\big)f(v)dv \;=\; -1+\zeta^2.$$

These in turn give that $\zeta^2+(1/E)\zeta-1=0$. Of the two roots to this equation, only one is possible if the energy $\int_{\mathbb{R}} v^2\,f(v)\,dv=1$, namely

$$\zeta \;=\; \frac{2E}{\sqrt{1+4E^2}+1}. \tag{2.80}$$

This gives the value of ζ in terms of E, the magnitude of the external force. We remark that, this value of ζ coincides with ζ_+ which was calculated in (2.23). Further, for any

$E > 0$, we see from (2.80) that $0 < \zeta < 1$, where in the limit $E \to \infty$ we have that $\zeta \to 1$ and in the limit $E \to 0$ we have that $\zeta \to 0$.

Using (2.79) in (2.76) results in

$$\left(\frac{1}{E} - \zeta\right) f(v) \;+\; \big(1 - \zeta\, v\big)\frac{d}{dv} f(v) \;=\; \frac{1}{E} Q^+(f,f)(v). \tag{2.81}$$

With the notations $\kappa = \frac{1}{\zeta}$ and $\gamma = \frac{1}{E\zeta} - 1$, equation (2.81) takes the form

$$\gamma\, f(v) \;-\; (v - \kappa) f'(v) \;=\; (\gamma + 1) Q^+(f,f)(v),$$

or, when $v \neq \kappa$,

$$f'(v) \;-\; \frac{\gamma}{v - \kappa}\, f(v) \;=\; -\frac{\gamma + 1}{v - \kappa}\, Q^+(f,f)(v).$$

We then find the integrating factor $|v - \kappa|^{-\gamma}$, so that

$$\frac{d}{dv}\left(\frac{1}{|v - \kappa|^{\gamma}}\, f(v)\right) \;=\; -\frac{\gamma + 1}{|v - \kappa|^{\gamma + 1}}\, Q^+(f,f)(v).$$

Any solution to (2.76), with $\int_{\mathbb{R}} f(v)\, dv = 1$ and $\int_{\mathbb{R}} v^2\, f(v)\, dv = 1$, satisfies

$$f(v) \;=\; \mathcal{A}(f)(v),$$

where $\mathcal{A}(f)(v)$ is defined by

$$\mathcal{A}(f)(v) \;=\; \frac{1}{|v - \kappa|} \int_{\mathbb{R}} \Phi\left(\frac{w - \kappa}{v - \kappa}\right) Q^+(f,f)(w) dw, \tag{2.82}$$

with $\Phi : \mathbb{R} \to [0, \infty)$ given by

$$\Phi(y) \;=\; \frac{\gamma + 1}{|y|^{\gamma + 1}} \mathbb{1}_{\{y > 1\}}(y).$$

The main result in Paper I is the following:

Theorem 2.4. *For all field strengths $E > 0$, the mapping $\mathcal{A}$ defined by (2.82) has a nonnegative fixed point f, which is a solution to (2.76)–the stationary Kac equation with a Gaussian thermostat. This solution satisfies*

(i) $\int_{\mathbb{R}} f(v) dv = 1$, $\int_{\mathbb{R}} v f(v) dv = \zeta$, *and* $\int_{\mathbb{R}} v^2 f(v) dv = 1$.

(ii) $\int_{\mathbb{R}} v^{2m} f(v) dv = C_{m,E}$, *for all positive integers m, where $C_{m,E}$ depends only on E and m. The value of these constants can be computed recursively.*

(iii) $f \in C\big(\mathbb{R} \setminus \{\kappa\}\big)$.

(iv) *For $E < \sqrt{2}$, $f \in C(\mathbb{R})$;*
for $E = \sqrt{2}$, f has a logarithmic singularity near $v = \sqrt{2}$; and
for $E > \sqrt{2}$, f has a singularity of the form $|v - \kappa|^\gamma$ near $v = \kappa$.

The result that, for $E < \sqrt{2}$, $f \in C(\mathbb{R})$ gives boundedness in $Q^+(f, f)$. This ceases to be the case if the field E is sufficiently large. We thus make some calculations to briefly study the behavior of $Q^+(f, f)$ at those points where f has power-like singularity. Towards this we recall that

$$Q^+(f,f)(v) \;=\; \int_{\mathbb{R}} \int_{-\pi}^{\pi} f(v')\, f(v'_*)\, \frac{1}{2\pi}\, d\theta\, dv_*,$$

where $v' = v\cos\theta - v_* \sin\theta$ and $v'_* = v\sin\theta + v_*\cos\theta$. By a change of variables, Q^+ can be rewritten as

$$Q^+(f,f)(v) \;=\; \int_{|v|}^{+\infty} g(r)\, \frac{r}{\sqrt{r^2 - v^2}}\, dr,$$

where

$$g(r) \;=\; \frac{1}{2\pi} \int_{-\pi}^{\pi} f(r\,\cos\theta)\, f(r\,\sin\theta)\, d\theta.$$

If $f(v) \sim |v - \kappa|^\gamma$ near $v = \kappa$, then

$$\begin{aligned} g(r) \;&>\; \int_{-\pi/8}^{\pi/8} |r\,\cos(\theta + \pi/4) - \kappa|^\gamma\, |r\,\sin(\theta + \pi/4) - \kappa|^\gamma\, d\theta \\ &=\; C \int_{-\pi/8}^{\pi/8} \left| \frac{r}{\sqrt{2}} \cos\theta - \frac{r}{\sqrt{2}} \sin\theta - \kappa \right|^\gamma \left| \frac{r}{\sqrt{2}} \sin(\theta) + \frac{r}{\sqrt{2}} \cos(\theta) - \kappa \right|^\gamma d\theta. \end{aligned}$$

This in turn gives

$$g(r) \;\sim\; \int_{-\pi/8}^{\pi/8} \Big| r\,\sin(\theta) - \big(r - \sqrt{2}\kappa\big) \Big|^\gamma \Big| r\,\sin(\theta) + \big(r - \sqrt{2}\kappa\big) \Big|^\gamma\, d\theta.$$

This finally makes $g(r) \sim \big| r - \sqrt{2}\,\kappa \big|^{1+2\gamma}$ near $r \sim \sqrt{2}\,\kappa$. With this we see that

$$\begin{aligned} Q^+\big(f,f\big)\big(\sqrt{2}\kappa\big) \;&\sim\; \int_{\sqrt{2}\kappa}^{R} |r - \sqrt{2}\,\kappa|^{1+2\gamma}\, \frac{r}{\sqrt{r^2 - 2\,\kappa^2}}\, dr \\ &=\; \int_{\sqrt{2}\kappa}^{R} \frac{|r - \sqrt{2}\,\kappa|^{\frac{1}{2}+2\gamma}\, r}{|r + \sqrt{2}\,\kappa|^{\frac{1}{2}}}\, dr, \end{aligned}$$

where R is large. This is integrable only when $\frac{1}{2} + 2\,\gamma > -1$, i.e. $\gamma > -\frac{3}{4}$. This in turn corresponds, from the definition of γ and the relation (2.80), to $E < 2\sqrt{5} \sim 4.47$.

2.6 Asymptotic solutions to the stationary problem

In this section we present a method of constructing an asymptotic solution to the stationary problem (2.76). This will enable us to study the effect of the force field on the behavior of the solution. If $E = 0$, then the solution to the stationary thermostatted Kac equation is the Maxwellian

$$M(v) \;=\; \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{v^2}{2}\right),$$

which is chosen to have unit mass and energy. For the Kac equation we necessarily have that $\int_{\mathbb{R}} v\, M(v)\, dv = 0$.

In this section, the field strength is denoted by ε, to indicate that it is relatively small. Then

$$\frac{d}{dv}\Big(\big(1-\zeta\, v\big)\, f(v)\Big) \;=\; \frac{1}{\varepsilon}\, Q(f,f)(v). \tag{2.83}$$

We may see this as fixing a time scale which is adapted to the field strength, and increasing the jump rate. For the Boltzmann equation it corresponds to decreasing the mean free path. A standard technique for studying the limit when $\varepsilon \to 0$ is the Hilbert expansion.

Having the form of the steady current ζ as a continuous function of $\varepsilon > 0$, given in (2.80), we perform a series expansion of type $\zeta = \sum_{k=1}^{\infty} \tilde{\zeta}_k\, \varepsilon^k$ for small values of ε and get

$$\zeta \;=\; \sum_{k=1;k\ \text{odd}}^{\infty} \binom{1/2}{(k+1)/2}\, 2^k\, \varepsilon^k, \tag{2.84}$$

where, for $r \in \mathbb{R}$, we use the usual combinatorial notation

$$\binom{r}{k} \;=\; \frac{r(r-1)\cdots(r-(k-1))}{k!}.$$

From (2.84) we deduce that $\zeta_0 = 0$, and for $k = 1, 2, 3, \ldots$

$$\tilde{\zeta}_k \;=\; \begin{cases} 0\,, & \text{for}\ \ k\ \ \text{even} \\ \displaystyle\binom{1/2}{(k+1)/2}\, 2^k, & \text{for}\ \ k\ \ \text{odd}. \end{cases} \tag{2.85}$$

We now look for a solution $f(v)$ to (2.76) in terms of a power series in ε:

$$f(v) \;=\; \sum_{k=0}^{\infty} \varepsilon^k\, f_k(v). \tag{2.86}$$

Corresponding to each of the terms in this sum we also introduce the quantities $e_k = \int_{\mathbb{R}} v^2 f_k(v)\,dv$, and note that $e_0 = 1$ and $e_k = 0$ for $k = 1, 2, 3, \ldots$. To be used in conjunction with these conditions is the result that $\int_{\mathbb{R}} v^m M(v)\,dv = 0$ for all odd m, and $\int_{\mathbb{R}} v^m M(v)\,dv > 0$ for all even m.

Inserting the formal series (2.86) in to the stationary equation (2.76) gives

$$\sum_{k=0}^{\infty} \varepsilon^k \left(\frac{d}{dv} f_k - \sum_{j=0}^{k} \zeta_{k-j} \left(f_j + v \frac{d}{dv} f_j \right) \right) = \sum_{k=0}^{\infty} \varepsilon^{k-1} Q_k, \tag{2.87}$$

where

$$\zeta_k = \int_{\mathbb{R}} v\, f_k(v)\,dv, \tag{2.88}$$

and for $k = 0, 1, 2, \ldots$

$$Q_k = \sum_{j=0}^{k} Q(f_j, f_{k-j}). \tag{2.89}$$

In this sum, we have the bilinear form associated with the operator Q

$$Q(f, g) = \frac{1}{2} \int_{\mathbb{R}} \int_{-\pi}^{\pi} \left(f'_* g' + f' g'_* - f_* g - f g_* \right) \frac{1}{2\pi} d\theta dv_*, \tag{2.90}$$

with the notation that $f_* \equiv f(v_*)$, $f'_* \equiv f(v'_*)$, $f' \equiv f(v')$, and $f \equiv f(v)$.

Multiplying both sides of (2.87) with v and integrating the resulting expressions over $\mathbb{R}$ with respect to v shows that ζ_k and $\tilde{\zeta}_k$ satisfy the same recursive relation, and therefore $\zeta_k = \tilde{\zeta}_k$.

Matching various orders in ε, we find a sequence of equations that can be solved recursively for f_k, similar to the Hilbert expansion of the Boltzmann equation. Accordingly, at the ε^{-1} level, we have that $Q(f_0, f_0) = 0$, which holds only if $f_0 = M$.

Rewriting (2.89) as

$$Q_k = Q(f_k, M) + Q(M, f_k) + \sum_{j=1}^{k-1} Q(f_j, f_{k-j}),$$

we note that $2\,Q(M, f_k)$ acts as a linear operator on the unknown f_k, while the remainder can be written as a source term, which we denote by $M\,S_{k-1}$. It is also convenient to put $f_k = M\,h_k$, with $h_0 = 1$, and to consider the h_k as the unknown. Thus Q_k takes the form

$$Q_k = M\,L\,h_k + M\,S_{k-1},$$

where the linearized collision operator L is given by

$$\begin{aligned} L\,h_k &= 2\,M^{-1}\,Q(M, Mh_k) \\ &= \int_{\mathbb{R}}\int_{-\pi}^{\pi} M_*\big(h'_{k*} + h'_k - h_{k*} - h_k\big)\,\frac{1}{2\pi}d\theta\,dv_*. \end{aligned} \tag{2.91}$$

Thus at the ε^k level, one obtains

$$\frac{d}{dv}f_k \;-\; \sum_{j=0}^{k-1}\zeta_{k-j}\left(f_j + v\,\frac{d}{dv}f_j\right) \;=\; M\,L\,h_{k+1} \;+\; M\,S_k, \tag{2.92}$$

which is equivalent to

$$-v\,h_k \;+\; \frac{d}{dv}h_k \;-\; \sum_{j=0}^{k-1}\zeta_{k-j}\left(h_j - v^2 h_j + v\,\frac{d}{dv}h_j\right) \;-\; S_k \;=\; Lh_{k+1}. \tag{2.93}$$

Here ζ_k is given by (2.85). Note that $\frac{d}{dv}\,(h_j\,M) = \big(\frac{d}{dv}h_j - v\,h_j\big)\,M$. Note also that, the sum in the left hand side of (2.93) runs up to $j = k-1$, because $\zeta_0 = 0$.

We see from (2.91) that L is self adjoint with respect to $M(v)\,dv$. Moreover

$$L\,h_k \;=\; 0 \text{ if and only if } h_k = a + bv^2, \quad a,\, b \in \mathbb{R},$$

i.e. $Ker(L) = \{a + b\,v^2 : a,\, b \in \mathbb{R}\}$.

It then follows that $L\,h_{k+1} = \varphi$ has a solution if and only if $\varphi \perp ker(L^*) = ker(L)$, i.e. if

$$\int_{\mathbb{R}} \varphi\,(a + b\,v^2)\,M(v)\,dv \;=\; 0.$$

The solution is unique up to a polynomial $\alpha + \beta\,v^2 \in ker(L)$. The Hilbert procedure consists in choosing α and β so that with $h_k \;+\; \alpha + \beta\,v^2$ inserted in to (2.93) makes the left hand side orthogonal to $Ker(L)$. It is then possible to solve for h_{k+1}, again modulo a polynomial in $ker(L)$.

The simple structure of the collision operator in the Kac equation makes it possible to perform very explicit calculations. We first note that, for a fixed non-negative integer m, if $g_m(v) = v^m$, then $Lg_m(v)$ is given by

$$\int_{\mathbb{R}}\int_{-\pi}^{\pi} M_*\left[\sum_{j=0}^{m}\binom{m}{j}v^{m-j}v_*^j\Big[(-1)^{m-j}\sin^{m-j}\theta\cos^j\theta + \cos^{m-j}\theta\sin^j\theta\Big] - v_*^m - v^m\right]\frac{d\theta}{2\pi}dv_*.$$

It then follows that,

$$\begin{aligned} Lg_m(v) &= -g_m(v), \text{ for all odd } m, \\ Lg_0(v) &= L\,g_2(v) = 0, \\ Lg_4(v) &= -\frac{1}{4}\big(v^4 - 6v^2 + 3\big), \\ Lg_6(v) &= -\frac{3}{8}\big(v^6 - 5v^4 - 15v^2 + 15\big), \text{ etc....} \end{aligned} \tag{2.94}$$

In fact,

$$\begin{aligned} Lg_{2i} &= \int_{\mathbb{R}}\int_{-\pi}^{\pi} M_*\, v^{2i}\left(\left(\sin^{2i}\theta + \cos^{2i}\theta\right) - 1\right)\frac{d\theta}{2\pi}dv_* + \text{lower order terms} \\ &= -\,v^{2i}\left(1 \;-\; \frac{1}{\pi}\int_{-\pi}^{\pi}\cos^{2i}\theta d\theta\right) + \text{lower order terms.} \end{aligned}$$

Moreover, $S_0 = 0$ and for $k = 2, 3, 4, \ldots$ we have

$$\begin{aligned} S_k &= M^{-1}\sum_{j=1}^{k} Q(Mh_j, Mh_{k-j+1}) \\ &= \frac{1}{2}\sum_{j=1}^{k}\int_{\mathbb{R}}\int_{-\pi}^{\pi} M_*\Big[h'_{j*}h'_{k-j+1} \;+\; h'_j h'_{k-j+1*} \\ &\qquad\qquad - \;h_{j*}h_{k-j+1} \;-\; h_j h_{k-j+1*}\Big]\frac{1}{2\pi}\,d\theta\, dv_*. \end{aligned} \tag{2.95}$$

Suppose now that, $h_k(v)$ is a polynomial of degree at most k, for $k \le k_0$:

$$h_k(v) = a_{k,k}\,v^k + a_{k,k-1}\,v^{k-1} + \ldots + a_{k,0}.$$

The left hand side of (2.93) is then a polynomial of degree at most $k+1 (k \le k_0)$, because S_k contains products of the form $h_j\,h_{k+1-j}$, and the sum in (2.93) runs up to $j = k-1$ only. The coefficient $a_{k+1,k+1}$ of v^{k+1} in h_{k+1} can now be determined uniquely. Similarly, all coefficients in the polynomial h_{k+1} can be determined, and so also h_{k_0+1} is a polynomial of degree at most $k_0 + 1$.

For $k = 1, 2, \ldots$, at each ε^k level of (2.93), we use the conditions on the e_k, and the form of S_k as given in (2.95), and determine, as an illustration, the first few terms of the unknown functions h_k:

$$\begin{aligned} h_k(v) &= 0, \quad \text{for all even } k, \\ h_1(v) &= v, \\ h_3(v) &= -v^3 + 2v, \\ h_5(v) &= v^5 - 6v^3 + 4v, \text{ etc....} \end{aligned}$$

We put these terms back in the setting of (2.86) with $f_k = Mh_k$, for $k = 1, 2, \ldots$, together with $f_0 = M$. This then gives the result that, for a small $\varepsilon > 0$

$$M(v)\Big(1 + \varepsilon v + \varepsilon^3\big(-v^3 + 2v\big) + \varepsilon^5\big(v^5 - 6v^3 + 4v\big) + \cdots\Big), \tag{2.96}$$

solves (2.76) asymptotically.

Part of this asymptotic solution is plotted in Figure 2.4 for some values of ε. Also depicted in Figure 2.4 is the behavior, as $\varepsilon \to 0$, of these non-equilibrium stationary solutions tending to the Maxwellian, thereby recovering the usual solution to the underlying Boltzmann equation. As shown in Figure 2.5 the truncated series may assume negative values which clearly is unphysical.

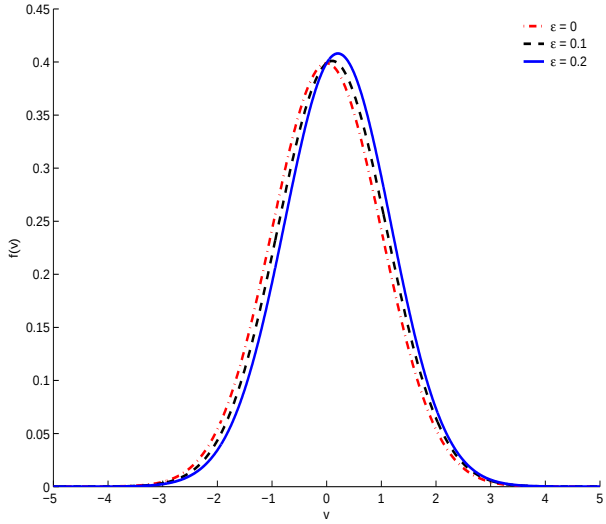

Figure 2.4: Asymptotic solution to the stationary problem according to (2.96) with external forces of relatively small magnitude.

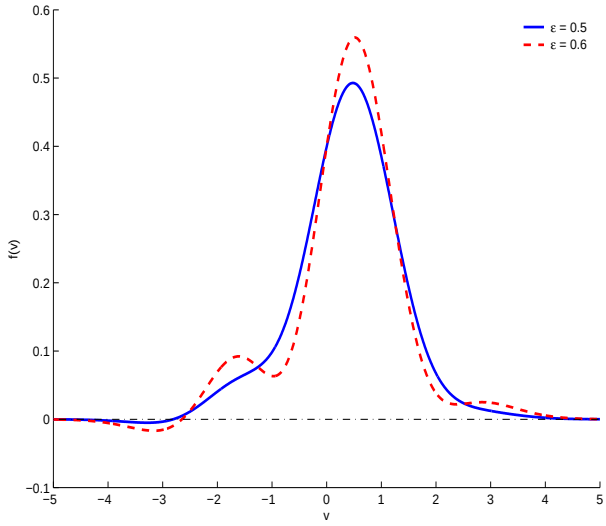

Figure 2.5: Use of external forces of slightly big magnitude in the asymptotic solution (2.96) causing unphysical result. More terms are needed in the expansion in order to get a good approximation.

Chapter 3

The Boltzmann equation with a Gaussian thermostat

In this chapter we consider the spatially homogeneous Boltzmann equation in the presence of an external force field and a Gaussian thermostat. Some of the questions that were studied for the Kac equation are addressed, although mostly on a formal level.

The first section describes the thermostatted particle system. The master equation governing the time evolution of the probability density of the three-dimensional velocities is presented. In the second section a formal derivation of the limiting Boltzmann equation is discussed. We make a closer look at the stationary equation in the final section of the chapter. In preparation for the numerical study in the next chapter, the major calculations are detailed for the special case where the force field is constant.

3.1 The thermostatted system

Consider a system of N velocities: $\mathbf{v}_i = (v_{i1}, v_{i2}, v_{i3}) \in \mathbb{R}^3$, $i = 1, 2, \ldots, N$. Let the corresponding 'master vector' $(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N) \in \mathbb{R}^{3N}$ be denoted by $\mathbf{V}$. We study the dynamics of such a system as the particles interact by random collisions while they are under the influence of an external force field $\mathbf{e} \in \mathbb{R}^3$ and in the presence of a Gaussian thermostat. Note that, one may consider the case where $\mathbf{e}$ is a function of velocity, i.e. $\mathbf{e} = \mathbf{e}(\mathbf{v})$. We denote by $\mathbf{E}$ the 'master field'

$$\mathbf{E} \;=\; \mathbf{E}(\mathbf{V}) \;=\; \big(\mathbf{e}(\mathbf{v}_1), \mathbf{e}(\mathbf{v}_2), \ldots, \mathbf{e}(\mathbf{v}_N)\big),$$

and for notational convenience we also write $\mathbf{e}_i = \mathbf{e}(\mathbf{v}_i)$, $i = 1, 2, \ldots, N$.

All the particles are accelerated by the field $\mathbf{e}$, and in order to keep the total energy, $\frac{1}{2}\sum_{i=1}^{N} |\mathbf{v}_i|^2$, constant, the 'master field' $\mathbf{E}$ must then be projected onto the tangent plane to the energy surface $\mathbb{S}^{3N-1}\big(\sqrt{N}\big)$ at the point $\mathbf{V}$. More precisely, between the jumps $\mathbf{V}$ evolves according to

$$\frac{d\mathbf{V}}{dt} \;=\; \mathbf{E} \;-\; \frac{\mathbf{E}\cdot\mathbf{V}}{|\mathbf{V}|^2}\mathbf{V} \;\equiv\; \mathbf{F}. \tag{3.1}$$

Here we use the shorthand notations $\mathbf{E}\cdot\mathbf{V} = \sum_{i=1}^{N} \mathbf{e}_i \cdot \mathbf{v}_i$ and $|\mathbf{V}|^2 = \sum_{i=1}^{N} |\mathbf{v}_i|^2$. The right hand side of (3.1) is the thermostatted master field, which, from now on, is denoted by $\mathbf{F}$.

Let $\mathbf{J} = \mathbf{J}(t)$ and $U = U(t)$ be defined by

$$\mathbf{J} \;=\; \frac{1}{N}\sum_{i=1}^{N} \mathbf{v}_i \;=\; (J_1, J_2, J_3), \tag{3.2}$$

$$U \;=\; \frac{1}{N}\sum_{i=1}^{N} |\mathbf{v}_i|^2. \tag{3.3}$$

If $\mathbf{e}$ is constant, then (3.1) may be written in terms of $\mathbf{J}$ and U as

$$\frac{d\mathbf{V}}{dt} \;=\; \mathbf{E} \;-\; \frac{\mathbf{e}\cdot\mathbf{J}}{U}\,\mathbf{V}. \tag{3.4}$$

Let $\alpha = (\mathbf{E}\cdot\mathbf{V})/|\mathbf{V}|^2$ and write (3.1) component-wise as $d\mathbf{v}_i/dt = \mathbf{e}_i - \alpha\,\mathbf{v}_i$. The dynamics of U is then given by

$$\begin{aligned}\frac{dU(t)}{dt} \;&=\; \frac{2}{N}\sum_{i=1}^{N} \mathbf{v}_i\cdot\big(\mathbf{e}_i - \alpha\,\mathbf{v}_i\big) \;=\; \frac{2}{N}\left(\sum_{i=1}^{N} \mathbf{v}_i\cdot\mathbf{e}_i \;-\; \alpha\sum_{i=1}^{N}|\mathbf{v}_i|^2\right) \;=\\ &=\; \frac{2}{N}\left(\mathbf{E}\cdot\mathbf{V} - \frac{\mathbf{E}\cdot\mathbf{V}}{|\mathbf{V}|^2}|\mathbf{V}|^2\right) \;=\; 0.\end{aligned}$$

This shows that U is constant in time, as it should be. It is, therefore, convenient to set $U = 1$. With this we can rewrite (3.1) component-wise as

$$\frac{d\mathbf{v}_i}{dt} \;=\; \mathbf{e}_i \;-\; \frac{1}{N}\big(\mathbf{E}\cdot\mathbf{V}\big)\,\mathbf{v}_i, \quad i = 1, 2, \ldots, N. \tag{3.5}$$

We note that, these equations are coupled via $\mathbf{E}(\mathbf{V})\cdot\mathbf{V}$.

If we restrict the calculations to the case where $\mathbf{e}$ is independent of $\mathbf{v}$, then without loss of generality we can write $\mathbf{e} = (\epsilon, 0, 0)$. There is then very little difference between the

one-dimensional and the three-dimensional cases. Equation (3.5) can, in this case, be expressed, component-wise, as

$$\begin{aligned} \frac{dv_{i1}(t)}{dt} \;+\; \epsilon\, J_1(t)\, v_{i1}(t) \;&=\; \epsilon, \\ \frac{dv_{i2}(t)}{dt} \;+\; \epsilon\, J_1(t)\, v_{i2}(t) \;&=\; 0, \\ \frac{dv_{i3}(t)}{dt} \;+\; \epsilon\, J_1(t)\, v_{i3}(t) \;&=\; 0, \end{aligned} \tag{3.6}$$

where $i = 1, 2, \ldots, N$. This can be solved explicitly, as soon as we have an exact expression for $J_1(t)$. This is treated in Chapter 4 where the explicit solutions are also used in the numerical simulations.

Let Ψ_N be a time-dependent probability density of the N three-dimensional velocities on $\mathbb{S}^{3N-1}$. In the presence of the external force field and with the introduction of the Gaussian thermostat, Ψ_N evolves in time according to

$$\frac{\partial}{\partial t}\Psi_N \;+\; \nabla\cdot\big(\mathbf{F}\;\Psi_N\big) \;=\; G\big(\Psi_N\big). \tag{3.7}$$

Here G is as given in (1.28), and $\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)$ is a shorthand notation for $\sum_{i=1}^{N}\frac{\partial}{\partial \mathbf{v}_i}\big[\mathbf{F}_i\,\Psi_N\big]$ with $\mathbf{F}_i = \mathbf{e}_i - \frac{1}{N}\big(\mathbf{E}\cdot\mathbf{V}\big)\mathbf{v}_i$. Equation (3.7) constitutes the master equation to the three-dimensional case and is analogous to (2.7). Using (3.5) we can also rewrite (3.7) as

$$\frac{\partial}{\partial t}\Psi_N(\mathbf{V},t) \;+\; \sum_{i=1}^{N}\frac{\partial}{\partial \mathbf{v}_i}\left(\left[\mathbf{e}_i \;-\; \frac{1}{N}\big(\mathbf{E}\cdot\mathbf{V}\big)\,\mathbf{v}_i\right]\Psi_N(\mathbf{V},t)\right) \;=\; G\big(\Psi_N\big)(\mathbf{V},t). \tag{3.8}$$

3.2 The limiting Boltzmann equation

Consider the three-dimensional master equation (3.7). We assume, throughout this section, that $\frac{1}{N}\sum_{i=1}^{N}|\mathbf{v}_i|^2 = 1$. For all fixed finite $k \in \mathbb{N}$, let the k-particle marginal f_k^N be defined by

$$f_k^N(\mathbf{v}_1,\ldots,\mathbf{v}_k,t) \;=\; \int_{\mathbb{S}^{3(N-k)-1}\left(\sqrt{N-\sum_{i=1}^{k}|\mathbf{v}_i|^2}\right)} \Psi_N(\mathbf{v}_1,\ldots,\mathbf{v}_N,t)\,d\boldsymbol{\sigma}_k, \tag{3.9}$$

where $d\boldsymbol{\sigma}_k(\mathbf{v}_{k+1},\dots,\mathbf{v}_N)$ is the surface element on $\mathbb{S}^{3(N-k)-1}\big(\sqrt{N-\sum_{i=1}^k|\mathbf{v}_i|^2}\big)$. Special cases of (3.9) are the one-particle marginal f_1^N and the two-particle marginal f_2^N:

$$f_1^N(\mathbf{v}_1,t)=\int_{\mathbb{S}^{3(N-1)-1}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\Psi_N(\mathbf{v}_1;\mathbf{v}_2,\dots,\mathbf{v}_N,t)\,d\boldsymbol{\sigma}_1,\ \text{and} \tag{3.10}$$

$$f_2^N(\mathbf{v}_1,\mathbf{v}_2,t)=\int_{\mathbb{S}^{3(N-2)-1}\left(\sqrt{N-|\mathbf{v}_1|^2-|\mathbf{v}_2|^2}\right)}\Psi_N(\mathbf{v}_1,\mathbf{v}_2;\mathbf{v}_3,\dots,\mathbf{v}_N,t)\,d\boldsymbol{\sigma}_2. \tag{3.11}$$

We recall that Ψ_N is said to have the Boltzmann property if

$$\lim_{N\to\infty}f_k^N(\mathbf{v}_1,\dots,\mathbf{v}_k,t)=\prod_{j=1}^k\lim_{N\to\infty}f_1^N(\mathbf{v}_j,t).$$

The main result of this section is

Theorem 3.1. *Suppose that $\Psi_N(\mathbf{v}_1,\dots,\mathbf{v}_N,t)$ is a sequence of C^1-solutions to (3.7) and that Ψ_N is symmetric in the variables $\mathbf{v}_1,\dots,\mathbf{v}_N$. If Ψ_N has the Boltzmann property, and if further*

$$f(\mathbf{v},t)\ =\ \lim_{N\to\infty}f_1^N(\mathbf{v},t),\ \textit{with}\ \int_{\mathbb{R}^3}f(\mathbf{v},t)\,d\mathbf{v}=1\ \textit{and}\ \int_{\mathbb{R}^3}|\mathbf{v}|^2\,f(\mathbf{v},t)\,d\mathbf{v}=1,$$

exists, then f satisfies the equation

$$\frac{\partial f}{\partial t}\ +\ div_{\mathbf{v}}\Big(\big(\mathbf{e}\ -\ \zeta_e(t)\,\mathbf{v}\big)f(\mathbf{v},t)\Big)\ =\ Q(f,f)(\mathbf{v},t), \tag{3.12}$$

where

$$\zeta_e(t)\ =\ \int_{\mathbb{R}^3}\mathbf{e}\cdot\mathbf{v}\,f(\mathbf{v},t)\,d\mathbf{v}, \tag{3.13}$$

and

$$Q(f,f)(\mathbf{v},t)\ =\ \int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\big(f(\mathbf{v}',t)f(\mathbf{v}'_*,t)-f(\mathbf{v},t)f(\mathbf{v}_*,t)\big)\frac{1}{4\pi}\,d\boldsymbol{\sigma}\,d\mathbf{v}_*. \tag{3.14}$$

Proof. We recall the result in Grünbaum[23] that, in the limit $N\to\infty$, the integral in the right hand side of (3.15) takes the form of $Q(f,f)$ as given in (3.14). His result is valid for the Boltzmann equation with no external force field. We *assume* that his result remains valid in the present situation. For the terms in the left hand side we carry out the proof for the general case where $\mathbf{e}=\mathbf{e}(\mathbf{v})$, and follow similar procedure as in the one-dimensional case.

We differentiate $f_1^N(\mathbf{v}_1,t)$ with respect to t and use (3.7) to get

$$\begin{aligned}\frac{\partial}{\partial t}f_1^N(\mathbf{v}_1,t) &= \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\frac{\partial}{\partial t}\Psi_N(\mathbf{v}_1;\mathbf{v}_2,\ldots,\mathbf{v}_N,t)d\boldsymbol{\sigma}_1\\ &= \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\Big(-\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)+G\big(\Psi_N\big)\Big)d\boldsymbol{\sigma}_1.\end{aligned}$$

This in turn can be written as

$$\frac{\partial}{\partial t}f_1^N(\mathbf{v}_1,t)+\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)d\boldsymbol{\sigma}_1 = \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}G\big(\Psi_N\big)d\boldsymbol{\sigma}_1. \quad (3.15)$$

Then the rest of the proof follows through the result of Lemma 3.1 which is presented next. ■

Lemma 3.1. *Let Ψ_N and f be as in Theorem 3.1. Let $\zeta(t)$ be as defined in (3.13). Let $\mathbf{F}$ be as given in (3.1). Then,*

$$\lim_{N\to\infty}\int_{S^{3N-1}(\sqrt{N})}\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)\;d\boldsymbol{\sigma}_0 \;=\; div_{\mathbf{v}}\Big(\big(\mathbf{e}\;-\;\zeta_e(t)\,\mathbf{v}\big)\,f\Big). \quad (3.16)$$

Proof. We carry out similar calculations like in the one-dimensional case. Let $\varphi=\varphi(\mathbf{v}_1)\in C_0^1(\mathbb{R}^3)$. For $r>0$, let $\eta_r=\eta_r(|\mathbf{V}|)$. This is to be taken as the characteristic function of the ball $\{\mathbf{V}:|\mathbf{V}|<r\}$. Then η_r is radial, so that $\nabla\eta_r\cdot\mathbf{F}=\sum_{i=1}^N\frac{\partial\eta_r}{\partial\mathbf{v}_i}\cdot\mathbf{F}_i=0$, where $\mathbf{F}_i=\mathbf{e}_i-\big(\frac{\mathbf{E}\cdot\mathbf{V}}{N}\big)\,\mathbf{v}_i$.

On the one hand, we have

$$\begin{aligned}&\int_{\mathbb{S}^{3N-1}(\sqrt{N})}\varphi(\mathbf{v}_1)\;\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\boldsymbol{\sigma}_0\\ &= \int_{|\mathbf{v}_1|<\sqrt{N}}\varphi(\mathbf{v}_1)\;\sqrt{\frac{N}{N-|\mathbf{v}_1|^2}}\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\boldsymbol{\sigma}_1\,d\mathbf{v}_1\\ &= \int_{\mathbb{R}^3}\varphi(\mathbf{v}_1)\;\sqrt{\frac{N}{N-|\mathbf{v}_1|^2}}\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)\,d\boldsymbol{\sigma}_1\,d\mathbf{v}_1, \quad (3.17)\end{aligned}$$

since φ has compact support in $\mathbb{R}^3$.

On the other hand, we formally have

$$\int_{\mathbb{S}^{3N-1}(\sqrt{N})}\varphi\;\nabla\cdot\big(\mathbf{F}\;\Psi_N\big)d\boldsymbol{\sigma}_0 \;=\; \frac{d}{dr}\left\{\int_{\mathbb{R}^{3N}}\eta_r\;\varphi\;\nabla\cdot\big(\mathbf{F}\,\Psi_N\big)d\mathbf{V}\right\}\Big|_{r=\sqrt{N}}. \quad (3.18)$$

Integration by parts gives

$$\int_{\mathbb{R}^{3N}} \eta_r\ \varphi\ \nabla\cdot\big(\mathbf{F}\ \Psi_N\big)d\mathbf{V} = -\int_{\mathbb{R}^{3N}} \nabla\big(\eta_r\ \varphi\big)\cdot\big(\mathbf{F}\ \Psi_N\big)d\mathbf{V}$$
$$= -\int_{\mathbb{R}^{3N}} \varphi\,\nabla\eta_r\cdot\big(\mathbf{F}\Psi_N\big)d\mathbf{V} - \int_{\mathbb{R}^{3N}} \eta_r\,\nabla\varphi\cdot\big(\mathbf{F}\Psi_N\big)\,d\mathbf{V}.$$

Since $\nabla\eta_r\cdot\mathbf{F}=0$, the first integral at the right hand side vanishes, and thus

$$\int_{\mathbb{R}^{3N}} \eta_r\ \varphi\ \nabla\cdot\big(\mathbf{F}\ \Psi_N\big)\ d\mathbf{V}\ =\ -\int_{\mathbb{R}^3}\frac{\partial\varphi}{\partial\mathbf{v}_1}\cdot\left\{\int_{\mathbb{R}^{3N-3}}\eta_r\ \mathbf{F}_1\ \Psi_N\ d\tilde{\mathbf{V}}\right\}d\mathbf{v}_1,$$

where $\mathbf{F}_1=\mathbf{F}_1(\mathbf{v}_1)=\mathbf{e}_1-\big(\frac{\mathbf{E}\cdot\mathbf{V}}{N}\big)\,\mathbf{v}_1$ is the first $\mathbb{R}^3$–component of the master field $\mathbf{F}$ and $d\tilde{\mathbf{V}}=d\mathbf{v}_2\,\ldots\,d\mathbf{v}_N$. Next we rewrite the inner integral as

$$\int_{\mathbb{R}^{3N-3}}\eta_r\ \mathbf{F}_1\ \Psi_N\,d\tilde{\mathbf{V}}=\int_0^{\sqrt{r^2-|\mathbf{v}_1|^2}}\left\{\int_{\mathbb{S}^{3N-4}(\rho)}\mathbf{F}_1\ \Psi_N\,d\boldsymbol{\sigma}_1\right\}d\rho.$$

Writing $\frac{1}{N}(\mathbf{E}\cdot\mathbf{V})=\frac{1}{N}\Big(\mathbf{e}_1\cdot\mathbf{v}_1+\sum_{i=2}^N\mathbf{e}_i\cdot\mathbf{v}_i\Big)$, the above integral can be rewritten as

$$\int_0^{\sqrt{r^2-|\mathbf{v}_1|^2}}\left\{\int_{\mathbb{S}^{3N-4}(\rho)}\left(\mathbf{e}_1-\frac{1}{N}\Big(\mathbf{e}_1\cdot\mathbf{v}_1+\sum_{i=2}^N\mathbf{e}_i\cdot\mathbf{v}_i\Big)\,\mathbf{v}_1\right)\ \Psi_N\,d\boldsymbol{\sigma}_1\right\}d\rho.$$

This in turn equals

$$\int_0^{\sqrt{r^2-|\mathbf{v}_1|^2}}\left\{\int_{\mathbb{S}^{3N-4}(1)}\left[\mathbf{e}_1-\frac{1}{N}\left(\mathbf{e}_1\cdot\mathbf{v}_1+\sum_{i=2}^N\mathbf{e}(\rho\,\boldsymbol{\omega}_i)\cdot\rho\,\boldsymbol{\omega}_i\right)\,\mathbf{v}_1\right]\ \Psi_N\,\rho^{3N-4}\,d\widetilde{\boldsymbol{\omega}}\right\}d\rho,$$

where $\widetilde{\boldsymbol{\omega}}=(\boldsymbol{\omega}_2,\ldots,\boldsymbol{\omega}_N)=\frac{1}{\rho}(\mathbf{v}_2,\ldots,\mathbf{v}_N)$. As in the case of the Kac equation, we differentiate with respect to r, and set $r=\sqrt{N}$, to get

$$\frac{\sqrt{N}}{\tilde{r}}\int_{\mathbb{S}^{3N-4}(1)}\left[\mathbf{e}_1-\frac{1}{N}\Big(\mathbf{e}_1\cdot\mathbf{v}_1+\sum_{i=2}^N\mathbf{e}\big(\tilde{r}\boldsymbol{\omega}_i\big)\cdot\boldsymbol{\omega}_i\Big)\,\mathbf{v}_1\right]\tilde{r}^{3N-4}\Psi_N\,d\widetilde{\boldsymbol{\omega}},$$

where $\tilde{r}=\sqrt{N-|\mathbf{v}_1|^2}$. This then takes the form

$$\sqrt{\frac{N}{N-|\mathbf{v}_1|^2}}\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\left(\mathbf{e}_1\ -\ \frac{1}{N}(\mathbf{E}\cdot\mathbf{V})\mathbf{v}_1\right)\Psi_N\,d\boldsymbol{\sigma}_1.$$

Using Lemma 3.2, which is stated and proved below, the above expression equals

$$-\int_{\mathbb{R}^3}\frac{\partial\varphi}{\partial\mathbf{v}_1}\left\{\sqrt{\frac{N}{N-|\mathbf{v}_1|^2}}\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)}\Big(\mathbf{e}_1\ -\ \frac{1}{N}(\mathbf{E}\cdot\mathbf{V})\mathbf{v}_1\Big)\Psi_N\,d\boldsymbol{\sigma}_1\right\}d\mathbf{v}_1.$$

This then converges, in the limit $N \to \infty$, to

$$-\int_{\mathbb{R}^3} \frac{\partial \varphi}{\partial \mathbf{v}_1} \Big(\big(\mathbf{e}_1 \ - \ \zeta_e(t)\, \mathbf{v}_1 \big)\, f(\mathbf{v}_1, t) \Big)\, d\mathbf{v}_1.$$

Integration by parts gives

$$\int_{\mathbb{R}^3} \varphi(\mathbf{v}_1)\, div_{\mathbf{v}_1} \Big(\big(\mathbf{e}_1 \ - \ \zeta_e(t)\, \mathbf{v}_1 \big)\, f(\mathbf{v}_1, t) \Big)\, d\mathbf{v}_1,$$

and comparing this with (3.17) gives the desired result, since φ is arbitrary. ■

Lemma 3.2. *Let Ψ_N and f be as in Theorem 3.1. Let $\zeta(t)$ be as defined in (3.13). Then,*

$$\lim_{N\to\infty} \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \left(\mathbf{e}_1 \ - \ \frac{1}{N} (\mathbf{E}\cdot\mathbf{V}) \mathbf{v}_1 \right) \ \Psi_N \ d\boldsymbol{\sigma}_1 \ = \ \Big(\mathbf{e}_1 \ - \ \zeta_e(t)\, \mathbf{v}_1 \Big)\, f(\mathbf{v}_1, t). \tag{3.19}$$

Proof: As in the previous proof we write $\frac{\mathbf{E}\cdot\mathbf{V}}{N} = \frac{1}{N}\mathbf{e}_1 \cdot \mathbf{v}_1 + \frac{1}{N}\sum_{i=2}^N \mathbf{e}_i \cdot \mathbf{v}_i$. Then we have

$$\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \frac{1}{N} (\mathbf{E}\cdot\mathbf{V})\, \mathbf{v}_1\, \Psi_N \ d\boldsymbol{\sigma}_1 \quad =$$

$$= \quad \frac{1}{N} \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} (\mathbf{e}_1 \cdot \mathbf{v}_1) \mathbf{v}_1 \Psi_N d\boldsymbol{\sigma}_1 \ +$$

$$+ \quad \frac{1}{N} \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \left(\sum_{i=2}^N \mathbf{e}_i \cdot \mathbf{v}_i \right) \mathbf{v}_1 \Psi_N d\boldsymbol{\sigma}_1.$$

This, due to the symmetry assumption on Ψ_N, equals

$$\frac{1}{N} (\mathbf{e}_1 \cdot \mathbf{v}_1) \mathbf{v}_1 \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \Psi_N d\boldsymbol{\sigma}_1 \ +$$

$$+ \quad \frac{N-1}{N} \mathbf{v}_1 \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} (\mathbf{e}_2 \cdot \mathbf{v}_2) \Psi_N d\boldsymbol{\sigma}_1,$$

which in turn equals

$$\frac{1}{N} (\mathbf{e}_1 \cdot \mathbf{v}_1) \mathbf{v}_1 f_1^N(\mathbf{v}_1, t) \ + \ \left(1 - \frac{1}{N} \right) \mathbf{v}_1 \int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} (\mathbf{e}_2 \cdot \mathbf{v}_2) \Psi_N d\boldsymbol{\sigma}_1.$$

Those terms with factor $1/N$ in the above sum vanish, in the limit $N \to \infty$. To study the remaining term, in the limit $N \to \infty$, we see that

$$\begin{aligned}
&\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \mathbf{e}_2 \cdot \mathbf{v}_2 \; \Psi_N \; d\boldsymbol{\sigma}_1 \;\; = \\
&= \int_{|\mathbf{v}_2|<\sqrt{N-|\mathbf{v}_1|^2}} \mathbf{e}_2 \cdot \mathbf{v}_2 \left(\sqrt{\frac{N-|\mathbf{v}_1|^2}{N-|\mathbf{v}_1|^2-|\mathbf{v}_2|^2}} \int_{\mathbb{S}^{3N-7}} \Psi_N \; d\boldsymbol{\sigma}_2 \right) d\mathbf{v}_2 \\
&= \int_{|\mathbf{v}_2|<\sqrt{N-|\mathbf{v}_1|^2}} \mathbf{e}_2 \cdot \mathbf{v}_2 \sqrt{\frac{N-|\mathbf{v}_1|^2}{N-|\mathbf{v}_1|^2-|\mathbf{v}_2|^2}} \; f_2^N(\mathbf{v}_1, \mathbf{v}_2, t) \; d\mathbf{v}_2. \qquad (3.20)
\end{aligned}$$

We rewrite (3.20) as

$$\begin{aligned}
&\int_{|\mathbf{v}_2|<\sqrt{N-|\mathbf{v}_1|^2}} \mathbf{e}_2 \cdot \mathbf{v}_2 f_1^N(\mathbf{v}_1, t) f_1^N(\mathbf{v}_2, t) d\mathbf{v}_2 \; + \\
&\int_{|\mathbf{v}_2|<\sqrt{N-|\mathbf{v}_1|^2}} \mathbf{e}_2 \cdot \mathbf{v}_2 \left[\sqrt{\frac{N-|\mathbf{v}_1|^2}{N-|\mathbf{v}_1|^2-|\mathbf{v}_2|^2}} f_2^N(\mathbf{v}_1, \mathbf{v}_2, t) - f_1^N(\mathbf{v}_1, t) f_1^N(\mathbf{v}_2, t) \right] d\mathbf{v}_2.
\end{aligned}$$

Under the assumption of molecular chaos, this converges, as $N \to \infty$, to

$$f(\mathbf{v}_1, t) \int_{\mathbb{R}^3} \mathbf{e}(\mathbf{v}_2) \cdot \mathbf{v}_2 \; f(\mathbf{v}_2, t) d\mathbf{v}_2$$

which takes the form $\zeta_e(t)\, f(\mathbf{v}_1, t)$. By assumption, we also have, as $N \to \infty$, that

$$\int_{\mathbb{S}^{3N-4}\left(\sqrt{N-|\mathbf{v}_1|^2}\right)} \mathbf{e}_1 \; \Psi_N \; d\boldsymbol{\sigma}_1 \;\; = \;\; \mathbf{e}_1 \, f_1^N(\mathbf{v}_1, t) \;\; \to \;\; \mathbf{e}_1 \, f(\mathbf{v}_1, t).$$

Thus the result in (3.19) follows. ■

3.3 The stationary equation

We consider (3.12) in the special case when $\mathbf{e} = (\epsilon, 0, 0)$ so that $(\mathbf{e} \cdot \mathbf{v})/|\mathbf{e}| = v_1$. Let also, for $i = 1, 2, 3$,

$$\zeta_i(t) \;\; = \;\; \int_{\mathbb{R}^3} v_i \, f(\mathbf{v}, t) d\mathbf{v}.$$

In the above case $\zeta_e(t) = \epsilon \, \zeta_1(t)$. Multiplying both sides of (3.12) by v_1 and then integrating with respect to $\mathbf{v}$ gives

$$\int_{\mathbb{R}^3} v_1 \, \frac{\partial f}{\partial t} d\mathbf{v} \;\; + \;\; \int_{\mathbb{R}^3} v_1 \, div_{\mathbf{v}} \Big(\big(\mathbf{e} - \epsilon \, \zeta_1(t) \, \mathbf{v} \big) \, f \Big) d\mathbf{v} \;\; = \;\; \int_{\mathbb{R}^3} v_1 \, Q(f, f)(\mathbf{v}, t) d\mathbf{v}. \qquad (3.21)$$

We recall that, for $i = 1, 2, 3$

$$\int_{\mathbb{R}^3} v_i \, Q(f,f)(\mathbf{v},t)\, d\mathbf{v} \;=\; 0,$$

and that

$$\begin{aligned}\int_{\mathbb{R}^3} v_1 \, div_{\mathbf{v}}\Big(\big(\mathbf{e} - \epsilon\,\zeta_1(t)\,\mathbf{v}\big)\, f\Big) d\mathbf{v} \;&=\; -\epsilon \int_{\mathbb{R}^3} f\, d\mathbf{v} \;+\; \epsilon\,\zeta_1(t) \int_{\mathbb{R}^3} v_1\, f\, d\mathbf{v} \\ &=\; -\epsilon \;+\; \epsilon\,\zeta_1(t)^2.\end{aligned}$$

From these observations, we see that (3.21) takes the form

$$\frac{d}{dt}\zeta_1(t) \;=\; \epsilon \;-\; \epsilon\,\zeta_1(t)^2.$$

In the same way, for $i = 2$ and $i = 3$, we have

$$\int_{\mathbb{R}^3} v_i \,\frac{\partial f}{\partial t} d\mathbf{v} \;+\; \int_{\mathbb{R}^3} v_i \, div_{\mathbf{v}}\Big(\big(\mathbf{e} - \epsilon\,\zeta_1(t)\,\mathbf{v}\big) f\Big) d\mathbf{v} = \int_{\mathbb{R}^3} v_i \, Q(f,f)\, d\mathbf{v},$$

so that

$$\frac{d}{dt}\zeta_i(t) \;=\; -\,\epsilon\,\zeta_1(t)\,\zeta_i(t),$$

which can also be solved to give

$$\zeta_i(t) \;=\; \zeta_i(0) \exp\left(-\,\epsilon \int_0^t \zeta_1(\tau) d\tau\right).$$

Thus we get the following system of differential equations

$$\frac{d}{dt}\zeta_1(t) \;=\; \epsilon \;-\; \epsilon\,\zeta_1(t)^2, \tag{3.22}$$

$$\frac{d}{dt}\zeta_2(t) \;=\; -\,\epsilon\,\zeta_1(t)\,\zeta_2(t), \tag{3.23}$$

$$\frac{d}{dt}\zeta_3(t) \;=\; -\,\epsilon\,\zeta_1(t)\,\zeta_3(t). \tag{3.24}$$

Given an initial data $\zeta_1(0)$, between -1 and $+1$, we solve (3.22) to get

$$\zeta_1(t) \;=\; \frac{C \;-\; \exp(-2\,\epsilon\,t)}{C \;+\; \exp(-2\,\epsilon\,t)},$$

where $C = \big(1 + \zeta_1(0)\big)/\big(1 - \zeta_1(0)\big)\big)$, so that

$$\begin{aligned}\zeta_1(t) \;&=\; \frac{1 \;+\; \zeta_1(0) \;-\; (1 - \zeta_1(0))\exp(-2\,\epsilon\,t)}{1 \;+\; \zeta_1(0) \;+\; (1 - \zeta_1(0))\exp(-2\,\epsilon\,t)} \\ &=\; \frac{\zeta_1(0)\,\cosh(\epsilon\,t) \;+\; \sinh(\epsilon\,t)}{\zeta_1(0)\,\sinh(\epsilon\,t) \;+\; \cosh(\epsilon\,t)}.\end{aligned} \tag{3.25}$$

Looking at (3.25) we note that $\zeta_1(t) \to 1$ as $t \to \infty$, and the limit is independent of ϵ.

Having the form of $\zeta_1(t)$ as in (3.25), and given initial data $\zeta_2(0)$ we solve (3.23) to get

$$\begin{aligned} \zeta_2(t) &= \frac{2\,\zeta_2(0)}{1 \;+\; \zeta_1(0) \;+\; (1-\zeta_1(0))\exp(-2\,\epsilon\,t)}\,\exp(-\epsilon\,t) \\ &= \frac{\zeta_2(0)}{\cosh(\epsilon\,t) \;+\; \zeta_2(0)\,\sinh(\epsilon\,t)}. \end{aligned} \tag{3.26}$$

Similarly, given $\zeta_3(0)$ we solve (3.24) and get

$$\zeta_3(t) \;=\; \frac{\zeta_3(0)}{\cosh(\epsilon\,t) \;+\; \zeta_3(0)\,\sinh(\epsilon\,t)}. \tag{3.27}$$

Here we also notice, respectively from (3.26) and (3.27), that $\zeta_2(t) \to 0$ and $\zeta_2(t) \to 0$ as $t \to \infty$.

These observations say that, for the special case $\mathbf{e} = (\epsilon, 0, 0)$, the current $\zeta(t) \to 1$ as $t \to \infty$. This shows that, in the limit $t \to \infty$, $\zeta(t)$ is independent of ϵ, contrary to the corresponding result for the modified Kac case. In fact, there are two different time scales involved: the collision frequency and a typical time scale for the accelerating field. While for the Kac equation, the collisions have an effect on the current ζ, this is not true for the Boltzmann equation, because $\int_{\mathbb{R}^3} \mathbf{v}\,Q(f,f)(\mathbf{v})\,d\mathbf{v} = 0$.

Thus the stationary case of (3.12) looks like

$$div_{\mathbf{v}}\Big(\big(\mathbf{e} \;-\; \epsilon\,\mathbf{v}\big)\,f(\mathbf{v})\Big) \;=\; Q(f,f)(\mathbf{v}).$$

An equivalent way of writing this is

$$\epsilon\,\frac{\partial f(\mathbf{v})}{\partial v_1} \;-\; 3\,\epsilon\,f(\mathbf{v}) \;-\; \epsilon\,\mathbf{v}\cdot grad_{\mathbf{v}} f(\mathbf{v}) \;=\; Q(f,f)(\mathbf{v}).$$

We finally note that if there are no collisions then the stationary solution is a Dirac mass at the point $(1,0,0)$. But this is a Maxwellian with zero temperature, and so this is still a solution when the collision term is added. And in fact,

$$\begin{aligned} \int_{\mathbb{R}^3} f(\mathbf{v},t)\big|\mathbf{v}-(1,0,0)\big|^2\,d\mathbf{v} &= \int_{\mathbb{R}^3} f(\mathbf{v},t)\left(|\mathbf{v}|^2 - 2\,v_1 + 1\right)\,d\mathbf{v} \\ &= 2 \;-\; 2\,\zeta_1(t) \;\to\; 0, \end{aligned}$$

when $t \to \infty$, and so the temperature goes to zero while the kinetic energy is conserved.

So from this point of view the stationary equation is much less interesting here than for the Kac equation, at least if one assumes uniqueness of the stationary state.

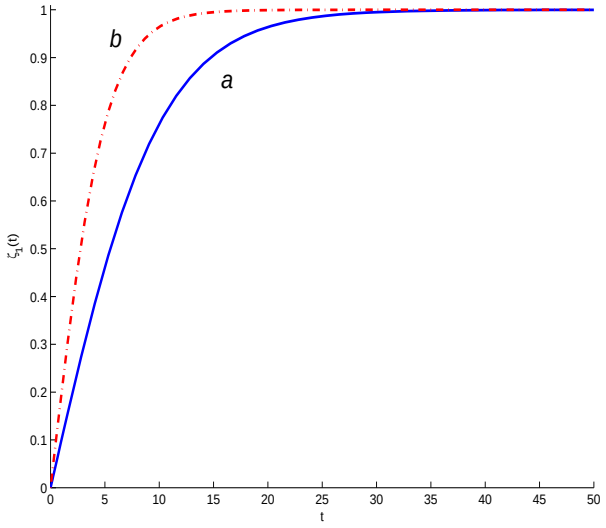

Figure 3.1: Explicit form of $\zeta_1(t)$ according to (3.25): (a) corresponds to $\epsilon = 0.1$ and (b) corresponds to $\epsilon = 0.2$. A change of field strength only changes the time scale. Collisions do not influence this result.

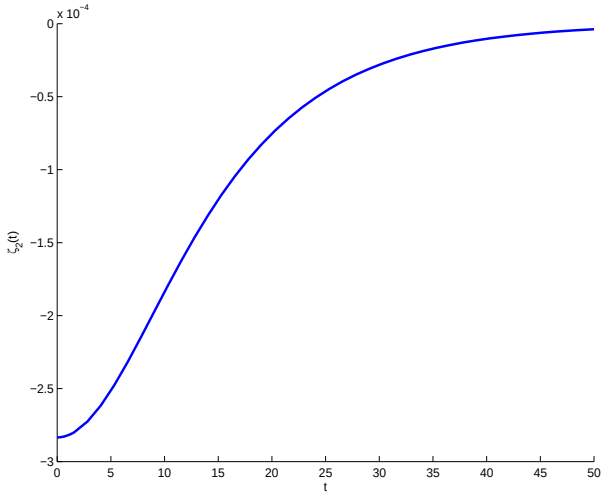

Figure 3.2: Explicit form of $\zeta_2(t)$ according to (3.26).

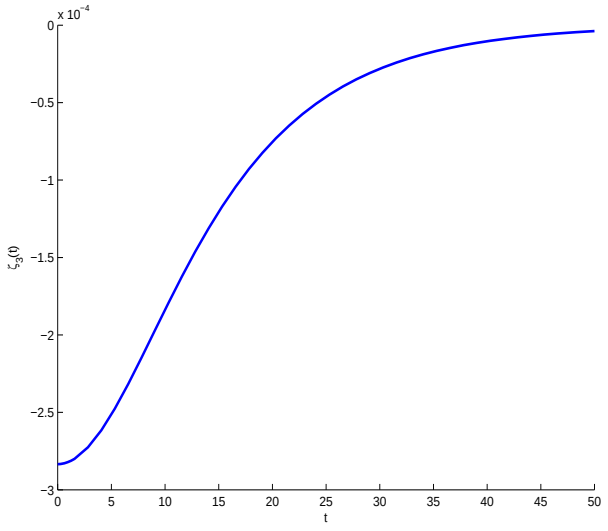

Figure 3.3: Explicit form of $\zeta_3(t)$ according to (3.27).

Chapter 4

Computational results

The mathematical difficulties involved in achieving exact analytical solutions on the one hand, and the need for practical calculations in rarefied gas dynamics on the other, have initiated the development of computational techniques to the Boltzmann equation. Simulation procedures, deterministic as well as stochastic types, of various levels of complexity have evolved along with the advent of powerful computers. Examples of the latter types are the Monte Carlo(MC) methods. Used mainly in statistical physics, MC methods have been serving as a means of simulating real physical processes using sequences of random numbers. The basis for MC simulations is to construct a suitable stochastic model in which the expected value of a certain random variable is equivalent to the value of the physical quantity to be determined. The expected value is then estimated by the average of many independent samples representing the random variable.

One variant of MC methods which has been widely employed for the modeling of rarefied gas flows is the Direct Simulation Monte Carlo(DSMC) method. Studies in rarefied gas dynamics require that calculations be performed at a molecular level, through the computation of the motion and collisions of representative molecules. The idea in implementing the DSMC method is to simulate a gas by letting a relatively small number of particles represent the whole gas. The collisions are simulated by assuming that the gas is homogeneous in a small space volume, and then to let all the particles in this volume evolve according to the stochastic processes similar to the models described in this thesis. Details and recent advances on the DSMC method, the underlying mathematical principles and its applications can be found, for e.g., in [3, 4, 11, 26].

In this chapter we present some numerical approximations of the stationary solutions to the thermostatted kinetic equations studied in the previous chapters. We are simulating a large number of trajectories to the jump processes defined on $\mathbb{S}^{N-1}\big(\sqrt{N}\big)$ and

$\mathbb{S}^{3N-1}(\sqrt{N})$, as described in Section 2.1 and Section 3.1 respectively. Following this brief introduction, we present some preliminary calculations where we give explicit formulas which are then used in the simulation. We then describe the method of simulations followed by discussion of the numerical results obtained.

4.1 Preliminary calculations

A random trajectory on $S^{N-1}(\sqrt{N})$ can be computed exactly thanks to the fact that there is an explicit solution to the evolution of the master vector $\mathbf{V}$ in between the jumps. Before discussing the results, we give these formulas, and describe the method of simulation.

For the one-dimensional velocities, we recall the definitions of J and U given in (2.3) and (2.4) respectively, and see that U is constant in time, while J evolves according to

$$\frac{dJ(t)}{dt} \;=\; E \;-\; \frac{E}{U}\,J(t)^2.$$

Having initial data $v_i(t_0)$, and thus $J_0 \equiv J(t_0)$, we solve for J at a later time t:

$$J(t) \;=\; \frac{J_0\cosh(\frac{E}{\sqrt{U}}t) \;+\; \sqrt{U}\sinh(\frac{E}{\sqrt{U}}t)}{\frac{J_0}{\sqrt{U}}\sinh(\frac{E}{\sqrt{U}}t) \;+\; \cosh(\frac{E}{\sqrt{U}}t)}\;.$$

The evolution in (2.1) can then be rewritten, component-wise, as the equations

$$\frac{dv_i(t)}{dt} + \frac{E}{U}J(t)v_i(t) = E, \qquad i = 1, 2, \ldots, N,$$

which have the solutions

$$v_i(t) \;=\; \frac{\sqrt{U}\sinh(\frac{E}{\sqrt{U}}t) \;+\; J_0\cosh(\frac{E}{\sqrt{U}}t) \;-\; J_0 \;+\; v_i(t_0)}{\cosh(\frac{E}{\sqrt{U}}t) \;+\; \frac{J_0}{\sqrt{U}}\sinh(\frac{E}{\sqrt{U}}t)}\;,\; i = 1, 2, \ldots, N. \quad (4.1)$$

This describes the velocity of each particle, under the influence of the external force, before any possible subsequent collision. We observe that, as time goes to infinity all the velocities concentrate at $\sqrt{U}$, namely that

$$v_i(t) \to \sqrt{U} \;\text{ as }\; t \to \infty.$$

We adapt these calculations to the 3-dimensional case. Recall the definitions of $\mathbf{J}$ and U as given in (3.2) and (3.3) respectively. As we have seen before U is constant in time,

thus we set $U = 1$. The dynamics of $\mathbf{J}$, in this special case, is

$$\begin{aligned}
\frac{d}{dt}J_1(t) &= \epsilon \; - \; \epsilon\, J_1(t)^2, \\
\frac{d}{dt}J_2(t) &= -\epsilon\, J_1(t)J_2(t), \\
\frac{d}{dt}J_3(t) &= -\epsilon\, J_1(t)J_3(t).
\end{aligned} \tag{4.2}$$

In the case where $\mathbf{e}$ depends on $\mathbf{v}$ one cannot, in a natural way, write a closed system of equations for the components of $\mathbf{J}$, and then it is also not possible to write separate equations for the components of $\mathbf{v}_i$ either, as we did in (3.6).

Given an initial state $\mathbf{V}(0)$, and thus $\mathbf{J}(0) = (J_1(0), J_2(0), J_3(0))$, we solve the system (4.2) at a later time $t > 0$, and get

$$\begin{aligned}
J_1(t) &= \frac{J_1(0)\,\cosh(\epsilon\, t) \; + \; \sinh(\epsilon\, t)}{J_1(0)\,\sinh(\epsilon\, t) \; + \; \cosh(\epsilon\, t)}, \\
J_2(t) &= J_2(0)\;\exp\Big(-\epsilon \int_0^t J_1(\tau)d\tau\Big), \\
J_3(t) &= J_3(0)\;\exp\Big(-\epsilon \int_0^t J_1(\tau)d\tau\Big).
\end{aligned}$$

With the explicit form of $J_1(t)$ available, the system in (3.6) is solved (for $i = 1, 2, \ldots, N$) to have the solutions

$$\begin{aligned}
v_{i1}(t) &= \frac{\sinh(\epsilon\, t) \; + \; J_1(0)\,\cosh(\epsilon\, t) - J_1(0) + v_{i1}(0)}{\cosh(\epsilon\, t) \; + \; J_1(0)\,\sinh(\epsilon\, t)}, \\
v_{i2}(t) &= \frac{v_{i2}(0)}{\cosh(\epsilon\, t) \; + \; J_1(0)\,\sinh(\epsilon\, t)}, \\
v_{i3}(t) &= \frac{v_{i3}(0)}{\cosh(\epsilon\, t) \; + \; J_1(0)\,\sinh(\epsilon\, t)}.
\end{aligned} \tag{4.3}$$

This gives the components of $\mathbf{v}_i$ as it moves under the influence of the external uniform force field $\mathbf{e} = (\epsilon, 0, 0)$ before it encounters any possible collision. In the limit $t \to \infty$, we see that $\mathbf{v}_i \to (1, 0, 0)$ and that only the rate of convergence depends on ϵ.

4.2 The algorithm

Next we briefly describe the algorithm used in the simulations. This is essentially the same for the one-dimensional velocities and the three-dimensional velocities. Fixed here are the initial distribution, the collision frequency, the terminal time, and N-the total number of velocities in the system.

i. Choose a waiting time randomly from an exponential distribution with rate proportional to N.

ii. Let all the v_i's evolve according to (4.1) during the chosen time interval.

iii. Perform collision:

   a. Choose a pair of indices i and j, $i \neq j$, randomly from $\{1, 2, \ldots, N\}$.

   b. Choose a collision parameter.

   c. Compute the post-collisional velocities v_i' and v_j' according to (1.13).

iv. Repeat this, until the terminal time is reached, with all random variables taken independently of the previous ones.

The only real difference between the two is the formula for computing the velocities after a collision. In adapting the above algorithm to the three-dimensional case we remark that the $\mathbf{v}_i$'s are to evolve according to (4.3), and the post-collisional velocities $\mathbf{v}_i'$ and $\mathbf{v}_j'$ are to be computed according to (1.3).

Remark 4.1. *Since the computational cost for each step is proportional to N (with a rather large proportionality factor, due to the complicated expression for the exact solution of the system of ODEs), and because the time interval between collisions is proportional to $1/N$, the total cost grows quadratically in N. Here we only use the simulations to illustrate the mathematical results, and hence we can afford to wait for the computations to finish. However, in real and practical situations, it would be necessary to devise a more efficient implementation.*

The simulation is also used to study the singular behavior of $Q^+(f, f)$ for the stationary solution f. We recall that

$$Q^+(f,f)(v) \;=\; \int_{\mathbb{R}} \int_{-\pi}^{\pi} f(v')\, f(v_*')\, \frac{1}{2\pi}\, d\theta\, dv_*.$$

For $v \in \mathbb{R}$, through a change of variables, we can rewrite $Q^+(f, f)(v)$ as

$$Q^+(f,f)(v) \;=\; \frac{1}{2\pi} \int_{\{u^2+u_*^2>v^2\}} \frac{1}{\sqrt{u^2+u_*^2-v^2}}\, f(u)\, f(u_*)\, du\, du_*. \tag{4.4}$$

To evaluate this integral by the algorithm described in Section 4.2, we let the process run until a stationary state is obtained. Then at stage (iii. c) of the algorithm, we save the resulting post-collisional velocities v_i' and v_j'. This gives a list of M collisional pairs $\{(u_m, u_{m*})\}_{m=1}^M$. The term $Q^+(f, f)(v)$ is then estimated as

$$\frac{1}{\pi\, M} \sum_{m=1}^{M} \frac{\mathbb{1}_{\{u_m^2+u_{m*}^2>v^2\}}}{\sqrt{u_m^2+u_{m*}^2-v^2}}, \tag{4.5}$$

a sum which is computed for a rather large number of values for v.

4.3 Results

We first present the results for the one-dimensional case in line with the modified Kac equation. In presenting the simulation results, it is illustrative to first look at the case $N = 3$. Having no force field ($E = 0$), Figure 4.1 shows the resulting one-particle marginal. Using the result that $|S^2(\sqrt{3})| = 12\pi$ in (1.22), and normalizing the resulting distribution then we get the constant one-particle marginal $f_1^3(v) = \frac{1}{2\sqrt{3}}$. This is in full agreement with the aforementioned simulation result. Figure 4.2 shows the distribution of phase points over the surface of the sphere $S^2(\sqrt{3})$, demonstrating the uniformity. Figure 4.3 and Figure 4.4 show the one-particle marginals obtained as we apply force fields of slightly higher magnitude on to the dynamics. We observe the slight departure from a uniform distribution.

The simulation also demonstrates the competition between the collision process, which tends to spread out phase points uniformly on the sphere, and the thermostatted force field, which tries to keep them concentrated at $(1, 1, 1)$ (for any N, $v_j(t) \to 1$ as $E\,t \to \infty$). For an extremely strong field E, we observe that the thermostatted field forces the most part of the density to concentrate at the point $(1, 1, 1)$ in the time interval between two collisions. The one-dimensional collision corresponds to a random rotation in a randomly chosen coordinate plane, and then the collisions would draw circles around the sphere, along the planes $v_j = 1$, $j = 1, 2, 3$. On the other hand, a very weak field would hardly move the particles between two collision events, and then the stationary distribution would remain almost uniform. Figure 4.5 shows an intermediary case, where the field is strong enough to indicate the concentration along the three circles $\{v_j = 1\} \cap S^2(\sqrt{3})$, $j = 1, 2, 3$.

Next we consider a large number of particles, and study the one-particle distribution. When N is sufficiently large, we expect the simulation result to approach $f(v)$, the stationary solution to (2.76). According to the theory, when the force field satisfies $E \geq \sqrt{2}$, the stationary solution has a singularity, and in the first simulation we study the limiting case $E = \sqrt{2}$ for a range of different N. A very large number of particles is needed to show the singularity. Figure 4.6 shows the one-particle marginal for simulations with varying N. The last one, with the highest peak corresponds to $N = 10^6$ and takes several hundred CPU-hours on a 2 GHz Pentium PC.

Figure 4.7 shows simulations for $E = \frac{9}{10}\sqrt{2}$, $E = \sqrt{2}$, and $E = \frac{11}{10}\sqrt{2}$. For 500 particles, one clearly sees how the maximum of the density moves with a varying field E, but it takes large N before one can begin to see the qualitative difference between fields smaller and bigger than $E = \sqrt{2}$. Figure 4.8 shows the densities for a bigger interval of f.

When $E \to \infty$, the stationary distribution should approach a Dirac mass at $v = 1$. Figure 4.9 shows how the density peaks for $E = 10\sqrt{2}$. The value of N used in that simulation is 10^4.

While these simulations show that a very large number of particles is needed to accurately demonstrate the singularity, a rather much smaller number of particles is enough if all that one is interested in is computing moments, $\int_{\mathbb{R}} v^j f(v)\,dv$. The last graph, Figure 4.10, shows the time evolution of the first few moments of the stationary solution f, for $E = \sqrt{2}$. The number of particles is 5000 which is more than sufficient to get an accurate estimation of the stationery values.

The results in Figures 4.11 – 4.14 show some observations on the behavior of $Q^+(f, f)$ for the stationary solution f of (2.76). To be noted here is that when the field is sufficiently strong ($E > 2\sqrt{5}$) then $Q^+(f, f)(v)$ displays a singularity at $|v| = \sqrt{2}\,\kappa$ as explained in Section 2.5. This implies that even though $f(v)$ is continuous except at $v = \kappa$, it is not C^1 as $f'(v)$ has a singularity at $|v| = \sqrt{2}\,\kappa$.

We have also done some simulations for the three-dimensional velocity case. This is done with $N = 5000$ and a force field of the form $\mathbf{e} = (0.1, 0, 0)$. The initial distribution is of the form

$$f_0(v_1, v_2, v_3) = \frac{1}{2}\big(\delta_{-0.5} + \delta_{0.5}\big)\,\frac{1}{2\pi}\exp\big(-\big(v_2^2 + v_3^2\big)\big).$$

In the result we notice that the majority of the velocities have first component close to 1 while the other two are close to zero. This is shown in the respective velocity-marginals in Figure 4.15 and Figure 4.16. The time evolution of $J_k = \frac{1}{N}\sum_{i=1}^{N} v_{ik}$, with $k = 1, 2, 3$, for this simulation are also shown in Figure 4.17. These results are to be compared with the exact solutions for $\zeta_k(t) = \int_{\mathbb{R}^3} v_k\, f(\mathbf{v}, t)\,d\mathbf{v}$ with $k = 1, 2, 3$, which were presented in Figures 3.1–3.3 in Section 3.3.

Results from the simulation showing the time evolution of the various moments of the solution $f(\mathbf{v}, t)$ are also presented in Figure 4.18. Those on the left correspond to $\int \varphi(\mathbf{v}) f(\mathbf{v}, t) d\mathbf{v}$ with $\varphi(\mathbf{v}) = v_1^2$, $\varphi(\mathbf{v}) = v_2^2$, and $\varphi(\mathbf{v}) = v_3^2$. Those on the right are similar results for $\varphi(\mathbf{v}) = v_1^2 + v_2^2 + v_3^2$ and $\varphi(\mathbf{v}) = v_1^4 + v_2^4 + v_3^4$.

Results for the one-dimensional case

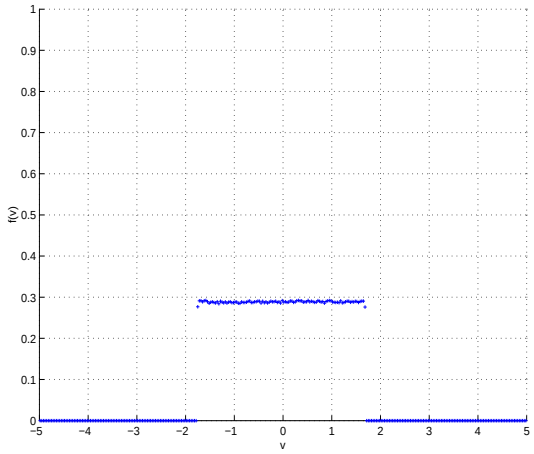

Figure 4.1: One-particle marginal $f_1^3(v)$ $(E = 0)$.

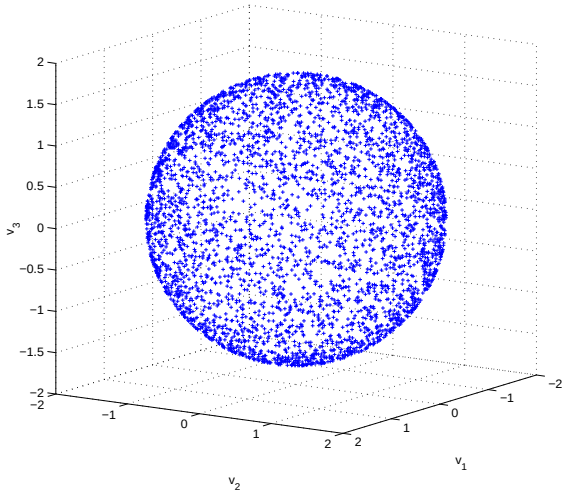

Figure 4.2: Uniform distribution of phase points on $S^2(\sqrt{3})$. $(N = 3, E = 0)$.

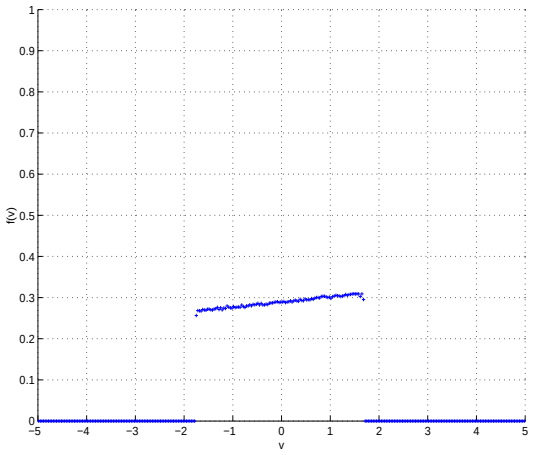

Figure 4.3: One-particle marginal $f_1^3(v)$ $(E = 0.1)$.

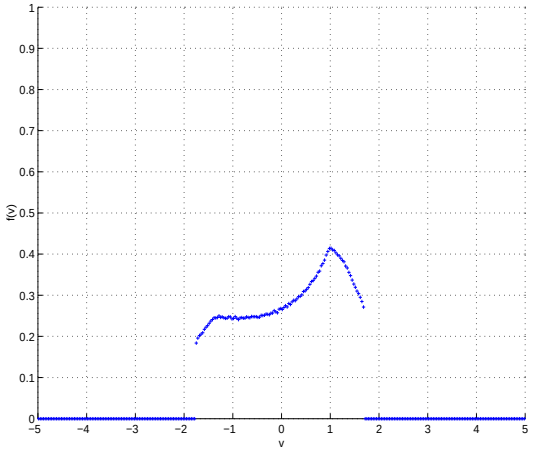

Figure 4.4: One-particle marginal $f_1^3(v)$ $(E = 0.5)$.

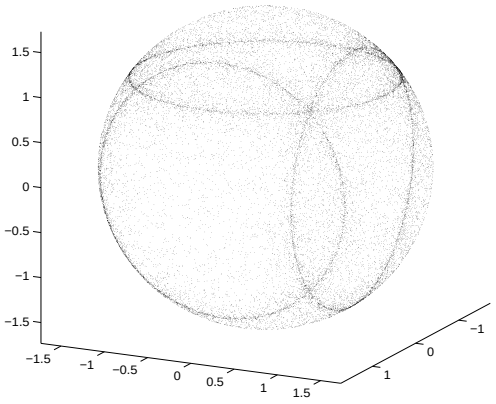

Figure 4.5: The stationary distribution of phase points on $S^2(\sqrt{3})$ for $N = 3$. Note the concentration along the circles $\{v_j = 1\} \cap \mathbb{S}^2(\sqrt{3})$, $j = 1, 2, 3$.

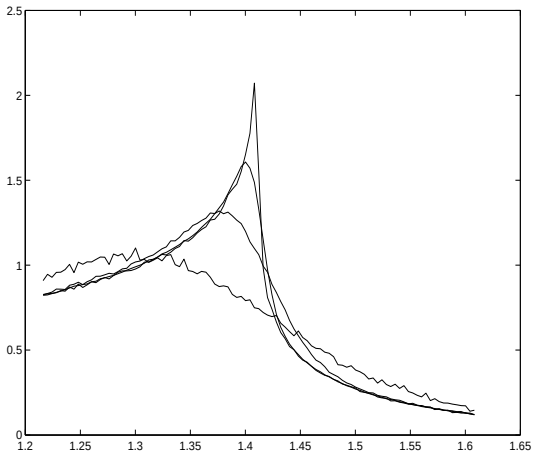

Figure 4.6: The stationary density $f(v)$; a close-up view near the singularity point $v = \kappa$. $E = \sqrt{2}$ (so $\kappa = \sqrt{2}$) and $N = 50; 500; 5000; 10^6$.

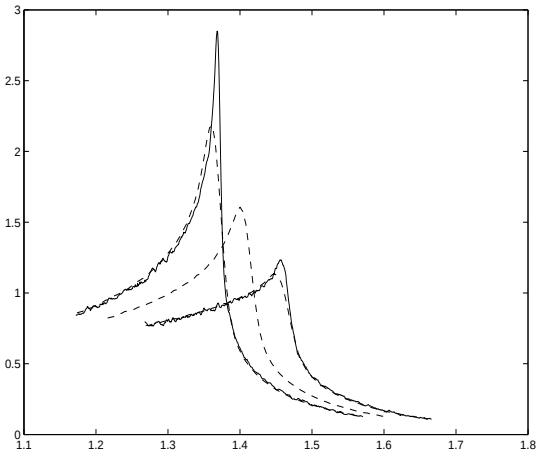

Figure 4.7: A closer view of the stationary state for $E = \frac{9}{10}\sqrt{2}$, $E = \sqrt{2}$, and $E = \frac{11}{10}\sqrt{2}$, near the singularity point, starting with the lowest curve. ($N = 5000$ (dashed line) and $N = 10^5$ (solid line)).

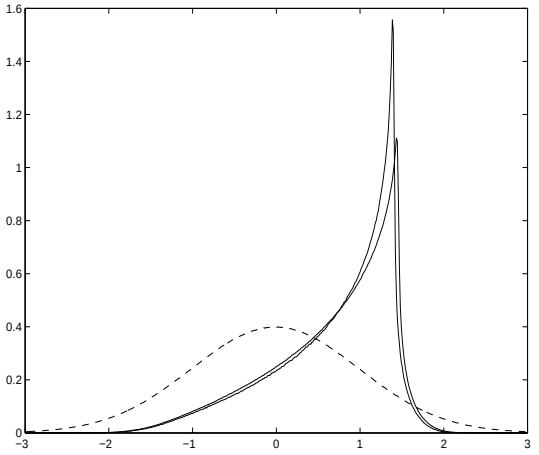

Figure 4.8: Stationary state for $E = \frac{9}{10}\sqrt{2}$ and $E = \sqrt{2}$, starting with the lowest curve; $N = 5000$. The dashed line shows the one-particle marginal for the uniform distribution on $S^{N-1}(\sqrt{N})$, which almost coincides with the Maxwellian.

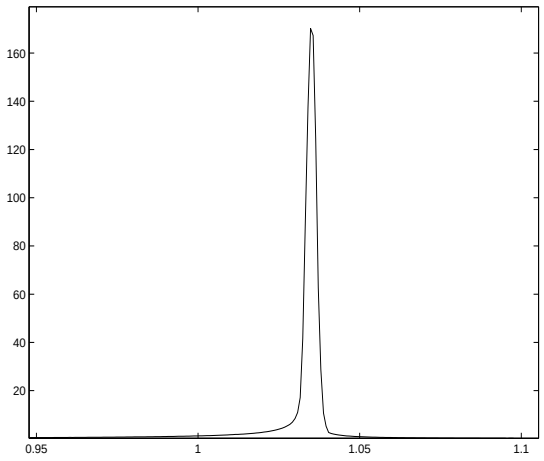

Figure 4.9: Stationary state for $E = 10\sqrt{2}$ with $N = 10000$, a close-up view near the singularity point $v = \kappa$.

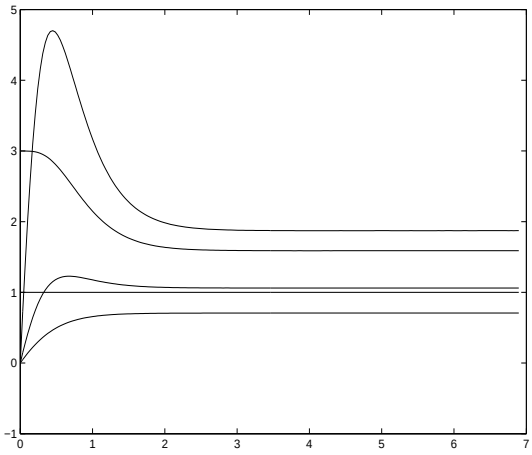

Figure 4.10: The evolution of moments, $\int_{\mathbb{R}} v^j \, f(v,t) \, dv$, $j = 1, 2, 3, 4, 5$, starting from the lowest curve. ($N = 5000$, $E = \sqrt{2}$.)

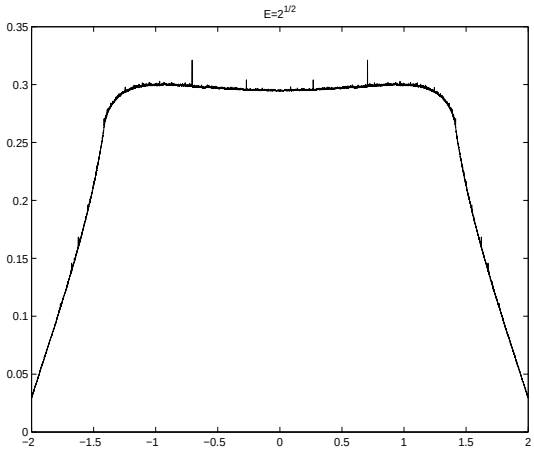

Figure 4.11: $Q^+(f,f)(v)$ for the stationary solution f of (2.76). $(N = 10000, E = \sqrt{2})$. The spikes in the graph are due to simulation noise.

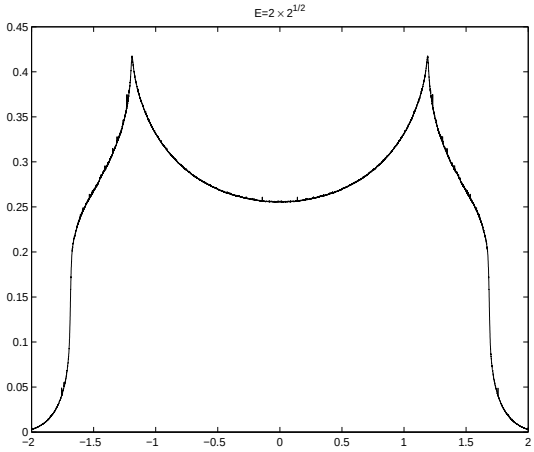

Figure 4.12: $Q^+(f,f)(v)$ for the stationary solution f of (2.76). $(N = 10000, E = 2\sqrt{2})$. (For $E = 2\sqrt{2}$, $\kappa \sim 1.1923$ and $\sqrt{2}\,\kappa \sim 1.6861$).

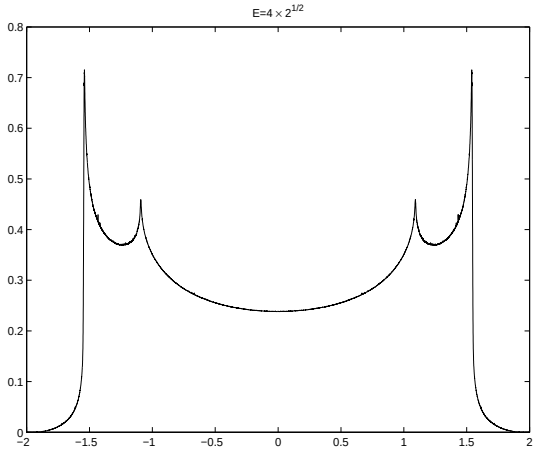

Figure 4.13: $Q^+(f,f)(v)$ for the stationary solution f of (2.76). ($N = 10000, E = 4\sqrt{2}$). Note that $Q^+(f,f)(v)$ shows singularities at $v = \kappa$ and $v = \sqrt{2}\,\kappa$. (For $E = 4\sqrt{2}$, $\kappa \sim 1.0923$ and $\sqrt{2}\,\kappa \sim 1.5447$).

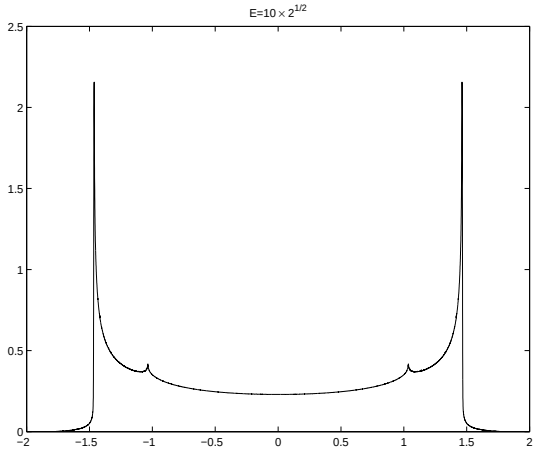

Figure 4.14: $Q^+(f,f)(v)$ for the stationary solution f of (2.76). ($N = 10000, E = 10\sqrt{2}$). Note that $Q^+(f,f)(v)$ shows singularities at $v = \kappa$ and $v = \sqrt{2}\,\kappa$. (For $E = 10\sqrt{2}$, $\kappa \sim 1.036$ and $\sqrt{2}\,\kappa \sim 1.465$).

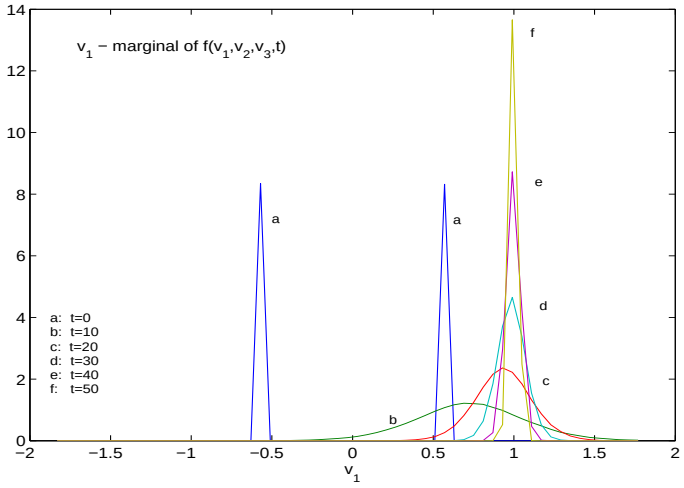

Figure 4.15: The v_1-marginal of $f(\mathbf{v},t)$: $\int_{\mathbb{R}} f(v_1,v_2,v_3,t)dv_2dv_3$ at $t = 0, 10, 20, 30, 40, 50$.

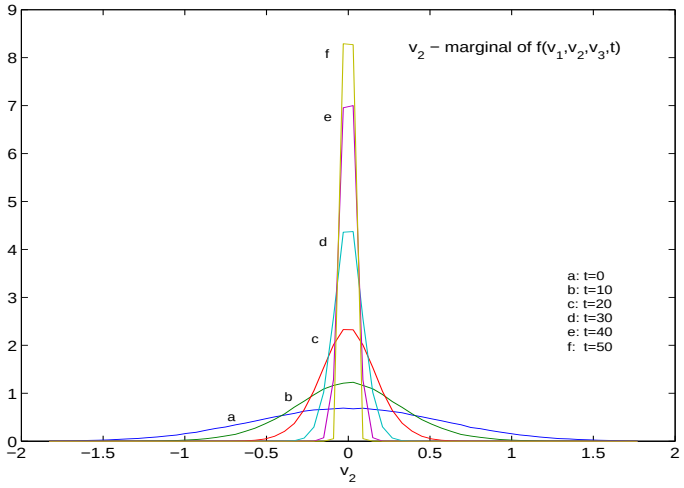

Figure 4.16: The v_2-marginal of $f(\mathbf{v},t)$: $\int_{\mathbb{R}} f(v_1,v_2,v_3,t)dv_1dv_3$ at $t = 0, 10, 20, 30, 40, 50$. Note that the v_3-marginal of $f(\mathbf{v},t)$ shows similar behavior.

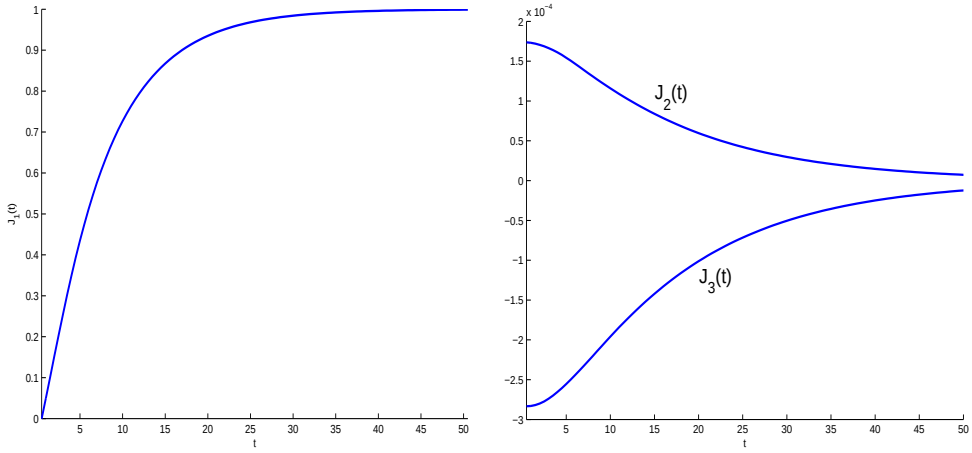

Figure 4.17: The time evolution of $J_1(t)$ (left), $J_2(t)$ and $J_3(t)$ (right).

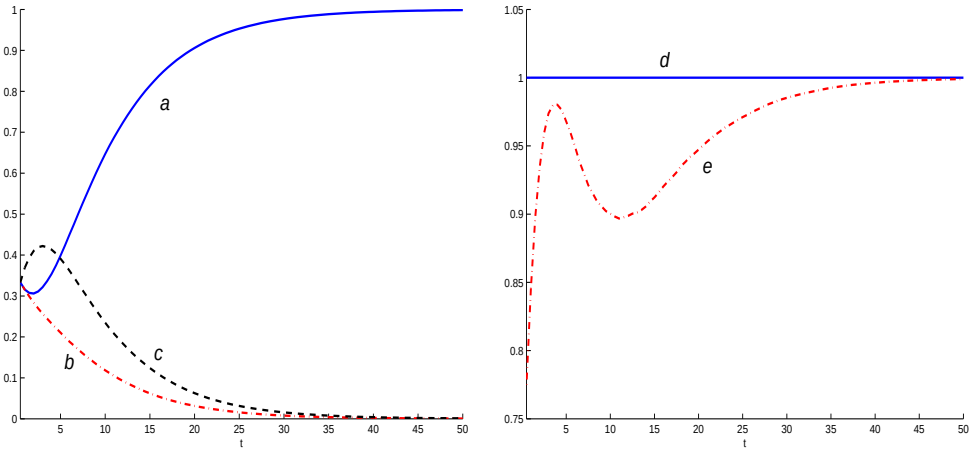

Figure 4.18: The time evolution of the various moments of $f(\mathbf{v},t)$: $\int \varphi(\mathbf{v})f(\mathbf{v},t)d\mathbf{v}$ where (on the left) (a) corresponds to $\varphi(\mathbf{v}) = v_1^2$, (b) to $\varphi(\mathbf{v}) = v_2^2$, (c) to $\varphi(\mathbf{v}) = v_3^2$. Similarly (on the right) (d) corresponds to $\varphi(\mathbf{v}) = v_1^2 + v_2^2 + v_3^2$, and (e) to $\varphi(\mathbf{v}) = v_1^4 + v_2^4 + v_3^4$.

Concluding Remarks

We finally mention the prospect for further developments in the direction of this study and briefly present some open problems.

1. In deriving the main equation studied in Chapter 2 we made a special assumption that the probability densities had to fulfill – the Boltzmann property. It is of great interest, therefore, to actually prove the propagation of molecular chaos in the presence of the thermostatted force field.

2. For the thermostatted Kac equation that we have studied, one would like to have stronger results regarding the long-time behavior of the solutions. One would like to prove that there is a unique stationary state, and that the unique solution to the time-dependent equation converges to this state as time tends to infinity. In that case it would also be interesting to find explicit rate estimates. The usual entropy arguments used in proving the trend to equilibrium do not work, as it is not immediate to find a natural candidate for the entropy functional in this case. It seems likely that a proof can be obtained via Fourier transform techniques. Work in this direction is in progress.

3. It would also be interesting to study the Kac collision term with more general collision cross sections. A non-cutoff cross section seems to eliminate the singularity of the stationary solution. This is also work in progress, in collaboration with Véronique Bagland.

4. In Chapter 3, concerning the Boltzmann equation, of course all of the above questions are still interesting, and they are not treated in this thesis. But many of the results that have been established for the Kac equation need to be solved for the Boltzmann equation as well. So for example, this thesis does not treat the existence and uniqueness problem for the Boltzmann equation with a thermostatted force field.

5. We have considered, in Chapter 3, that the force field that may depend on the velocity, and the limiting Boltzmann equation is derived with this possibility. It

would, therefore, be interesting to see what kind of force field would be needed to grant more interesting stationary situations.

6. If this kind of problem would appear in a situation where real numerical simulations are necessary, then one would need to find a more efficient way of doing the simulations. In particular it is less efficient to use the explicit solution of the system of ODE's to update the velocities between the collisions.

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Paper I *

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