Thesis for the Degree of Licentiate of Philosophy

Kac's Master Equation with a Gaussian Thermostat

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Abstract

In a first successful attempt to rigorously derive the Boltzmann equation from a many-particle system, M. Kac introduced a stochastic model, in which particle velocities make jumps due to random interactions between pairs of particles.

In this thesis, we introduce a related model where the particles, in addition to the random collisions, are accelerated by a uniform force field. The energy supplied is absorbed by a so called Gaussian thermostat, which keeps the total kinetic energy constant. We derive the master equation, which governs the dynamics of the system, and the corresponding Boltzmann equation. The latter describes the time evolution of the single-particle distribution function in the limit of infinitely many particles. We also study the non-equilibrium stationary states of this equation. In a particular case, it is shown that, such a state has a singularity. Computational results using a Monte Carlo method are also presented.

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

2000 Mathematics Subject Classification: Primary 76P05, 82B40; Secondary 45K05, 60C05, 60Gxx, 70Fxx.

Contents

Chapter 1

Introduction

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 represented by the distribution function $f \equiv f(\mathbf{x}, \mathbf{v}, t)$ of its molecules over the space coordinate $\mathbf{x} \in \mathbb{R}^3$ and velocity $\mathbf{v} \in \mathbb{R}^3$. The time evolution of f is governed by the Boltzmann equation

$$\partial_t f \;+\; \mathbf{v} \cdot \nabla_{\mathbf{x}} f \;+\; \mathbf{E} \cdot \nabla_{\mathbf{v}} f \;=\; Q(f, f) \;, \tag{1.1}$$

where the gradient operators $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{v}}$ denote derivatives with respect to the space variable $\mathbf{x}$ and the velocity $\mathbf{v}$ respectively. $\mathbf{E} \equiv \mathbf{E}(\mathbf{x}, \mathbf{v})$ denotes an external force per unit mass acting on a particle at position $\mathbf{x}$ having velocity $\mathbf{v}$, and the $\cdot$ denotes the Euclidean inner product in $\mathbb{R}^3$.

The term Q, on the right hand side, is a non-linear integral operator, which describes the collisions involved and acts only on the velocity dependence of f. It is defined by

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

with the notation that $f' \equiv f(\mathbf{x}, \mathbf{v}', t)$, $f'_* \equiv f(\mathbf{x}, \mathbf{v}'_*, t)$, and $f_* \equiv f(\mathbf{x}, \mathbf{v}_*, t)$.

The post-collisional molecular velocities, denoted by $\mathbf{v}'$ and $\mathbf{v}'_*$, are related to the respective pre-collisional molecular velocities $\mathbf{v}$ and $\mathbf{v}_*$ and to the collision parameter $\boldsymbol{\sigma}$ via the relation

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

where $\boldsymbol{\sigma}$, on the centre-of-mass frame of reference, varies over $\mathbb{S}^2$ - the unit sphere in $\mathbb{R}^3$. In Eq. 1.2, $d\boldsymbol{\sigma}$ denotes the normalised surface measure on $\mathbb{S}^2$ and $d\mathbf{v}_*$ denotes the Lebesgue measure on $\mathbb{R}^3$. Further, the collision kernel B is a non-negative function whose exact form depends on the intermolecular force law which specifies the particular molecular model. Details can be obtained in [11, 12, 13, 29].

Just to mention one important model in dimension 3, let the scattering angle θ be such that $\cos\theta = \frac{\mathbf{v}-\mathbf{v}_*}{|\mathbf{v}-\mathbf{v}_*|}\cdot\boldsymbol{\sigma}$, and consider an intermolecular force which varies like r^{-s}, where r denotes the intermolecular distance, and $s > 2$. In this case the collision kernel B takes the form

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

where $\alpha = \frac{s-5}{s-1}$, and b is a non-elementary function which behaves like $\frac{K}{|\theta|^{\alpha}}$, for θ close to 0, where $K > 0$. Since $\alpha > 1$, this singularity in the angular variable θ is always non-integrable. To overcome this difficulty, Grad introduced an angular cutoff near $\theta = 0$. This is to consider the form of B as in Eq. 1.4 where b is such that $\theta \mapsto \sin\theta\; b(\cos\theta)$ is integrable near $\theta = 0$.

The special case $s = 5$, or equivalently $\alpha = 0$, where the dependence on $|\mathbf{v}-\mathbf{v}_*|$ vanishes, corresponds to what is known as Maxwell molecules.

Let $\phi = \phi(\mathbf{v})$ be any, sufficiently regular, function. If f and ϕ are such that the indicated integrals exist, the collision integral $Q(f,f)$ fulfils

$$\int_{\mathbb{R}^3} Q(f,f)(\mathbf{v})\phi(\mathbf{v})\, d\mathbf{v} \;=\; \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \left(\phi'_* + \phi' - \phi_* - \phi\right) f\, f_*\, B\, d\boldsymbol{\sigma}\, d\mathbf{v}_*\, d\mathbf{v} \;. \tag{1.5}$$

Conservation of mass, momentum and energy at the level of the Boltzmann operator is recovered by taking $\phi(\mathbf{v}) = 1,\ \mathbf{v},\ \frac{1}{2}|\mathbf{v}|^2$ in Eq. 1.5:

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

Another fundamental property of the Boltzmann equation is the H-theorem. Define the H-function by

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

Boltzmann's H-theorem states that $\dfrac{dH(t)}{dt} \le 0$, saying that H can never increase with time. The equality sign holds only for the Maxwellian distribution function M, which describes an equilibrium state of the gas. The form of this Maxwellian is

$$M(\mathbf{v}) \;=\; \left(\frac{m}{2\,\pi\, k\, T}\right)^{\frac{3}{2}} \exp\left(-\,\frac{m\,|\mathbf{v}-\mathbf{u}|^2}{2\, k\, T}\right) \;,$$

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

1.2 Kac's Model of the Boltzmann Equation

In view of the great theoretical difficulties in studying the Boltzmann equation, Kac introduced a model equation by considering particles with one-dimensional velocities, and are uniformly distributed in configuration space. Further, b takes the form $b(\cos\theta) = \frac{1}{2\pi}$, i.e. the scattering angle θ is uniformly distributed over $[0, 2\pi)$. The resulting Boltzmann equation, also referred to as Kac's equation, describing the time evolution of the velocity distribution function f of a single particle, is then

$$\partial_t f(v,t) \;=\; Q(f,f)(v,t) \;, \tag{1.6}$$

where

$$Q(f,f)(v,t) \;=\; 2\int_{-\infty}^{+\infty}\int_0^{2\pi} \Big(f(v',t)f(v'_*,t) - f(v,t)f(v_*,t)\Big)\, \frac{1}{2\pi}\, d\theta\, dv_* \;, \tag{1.7}$$

and the post-collisional velocities v' and v'_* are given by

$$\begin{aligned} v' &= \quad v\cos\theta \;+\; v_*\sin\theta \\ v'_* &= -\,v\sin\theta \;+\; v_*\cos\theta \;. \end{aligned} \tag{1.8}$$

It is this equation, with some variations, that constitutes the thesis of this work.

An exact solution to Eq. 1.6 with a particular type of initial distribution is discussed in Ernst [15] and is given by

$$f(v,t) \;=\; \frac{1}{2C^{\frac{3}{2}}}\Big(\frac{3}{2}(C-1) + (3-C)\frac{v^2}{C^2}\Big)\exp\big(-\frac{v^2}{C}\big) \;, \tag{1.9}$$

where $C \equiv C(t)$ is given by $C(t) = 3 - 2\exp\big(-\frac{\sqrt{\pi}}{16}t\big)$.

This special solution is obtained solely due to the underlying symmetry of the Boltzmann equation for Maxwell molecules. This has been thoroughly investigated by Bobylev in [7]. The time evolution of this solution is shown in Figure 1.1.

A rigorous derivation of the non-linear Boltzmann equation Eq. 1.6 from a microscopic linear model was carried out by Kac in [21]. He considered a gas consisting of N point particles having one-dimensional velocities and interact through random binary collisions which happens at random times. The velocities are denoted by $v_i \in \mathbb{R}$ for $i = 1, 2, \ldots, N$; and are combined into a *master vector* $\mathbf{V} \equiv (v_1, v_2, v_3, \ldots, v_N) \in \mathbb{R}^N$. The stochastic dynamics is such that given an initial state $\mathbf{V}(0)$, at a random time a collision occurs between randomly chosen particles. This results in a jump in the state of the system. At any given instant $t > 0$, the collision mechanism keeps the total kinetic energy constant, say $\sum_{i=1}^N v_i^2 = N$. This makes $\mathbf{V}(t)$ a random variable with values in $\mathbb{S}^{N-1}(\sqrt{N})$, the sphere in $\mathbb{R}^N$ of radius $\sqrt{N}$.

The time intervals between successive collisions are assumed to be independent and exponentially distributed with mean duration $\tau_N > 0$, i.e. the probability that a collision happens later than time $t > 0$ after the previous collision is given by $\exp(-\frac{t}{\tau_N})$.

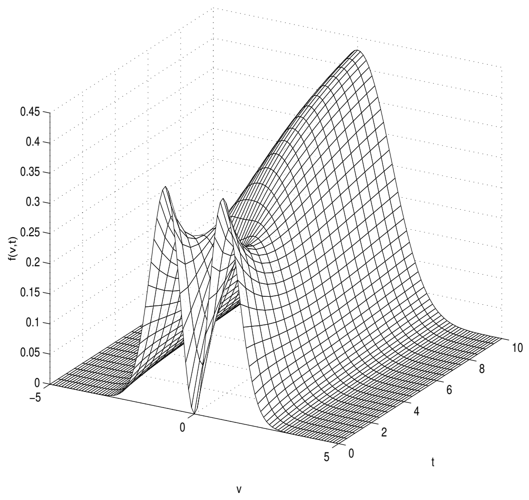


Figure 1.1: Evolution of an exact solution to Kac's equation.

Next we specify the evolution of this many-particle system. To this end, consider ψ_N, a continuous function on $\mathbb{R}^N \times [0,\infty)$, and its restriction on $\mathbb{S}^{N-1}(\sqrt{N}) \times [0,\infty)$. Define the operator $\tilde{K}$ by

$$\tilde{K}(\psi_N)(\mathbf{V},t) = \frac{1}{\binom{N}{2}} \sum_{1\le i<j\le N} \frac{1}{2\pi}\int_0^{2\pi} \psi_N\left(A_{ij}(\theta)\mathbf{V},t\right) d\theta \ , \tag{1.10}$$

where the $A_{ij}(\theta)$ are rotations by an angle θ on the v_iv_j plane:

$$A_{ij}(\theta)\mathbf{V} = (v_1,\ldots,v_i\cos\theta + v_j\sin\theta,\ldots,-v_i\sin\theta+v_j\cos\theta,\ldots,v_N) \ . \tag{1.11}$$

The probability density ψ_N of the N velocities at time t is then fully determined as the solution of the equation

$$\partial_t\psi_N(\mathbf{V},t) = K(\psi_N)(\mathbf{V},t) \tag{1.12}$$

where the operator K is given by

$$\begin{aligned} K(\psi_N)(\mathbf{V},t) &= N(\tilde{K}-I)(\psi_N)(\mathbf{V},t) \\ &= \frac{2}{N-1}\sum_{1\le i<j\le N}\frac{1}{2\pi}\int_0^{2\pi}\Big(\psi_N(A_{ij}(\theta)\mathbf{V},t)-\psi_N(\mathbf{V},t)\Big)\, d\theta \ , \end{aligned} \tag{1.13}$$

with the $A_{ij}(\theta)$ as given in Eq. 1.11.

Eq. 1.12, describing the joint evolution of the N velocities, is what is known as Kac's master equation. A related many-particle system, with 3-dimensional velocities, and the resulting Boltzmann equation was studied in Grünbaum [17]. This study was extended and given a more algebraic flavour in McKean [20, 19].

One major assumption in Kac's derivation is that, for each N, ψ_N is symmetric in the $v_1, v_2, \ldots, v_N$ variables. Physically, this corresponds to the assumption of indistinguishable particles in the system. For all fixed finite k, define the k-particle marginal f_k^N by

$$f_k^N(v_1,\ldots,v_k,t) = \int_{\mathbb{S}^{N-1-k}\left(\sqrt{N-v_1^2-\cdots-v_k^2}\right)} \psi_N(v_1,\ldots,v_k;v_{k+1},\ldots,v_N,t)\,d\sigma_k \ , \tag{1.14}$$

where $d\sigma_k \equiv d\sigma_k(v_{k+1},\ldots,v_N)$ denotes the surface element on $\mathbb{S}^{N-1-k}\left(\sqrt{N-v_1^2-\cdots-v_k^2}\right)$. Special cases are the single-particle marginal f_1^N and the two-particle marginal f_2^N which are given respectively by

$$f_1^N(v_1,t) = \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} \psi_N(v_1;v_2,\ldots,v_N,t)\,d\sigma_1 \ , \tag{1.15}$$

$$f_2^N(v_1,v_2,t) = \int_{\mathbb{S}^{N-3}\left(\sqrt{N-v_1^2-v_2^2}\right)} \psi_N(v_1,v_2;v_3,\ldots,v_N,t)\,d\sigma_2. \tag{1.16}$$

Differentiating both sides of Eq. 1.15 with respect to t, using Eq. 1.12 and the form of K as given in Eq. 1.13 yields

$$\begin{aligned}\partial_t f_1^N(v_1,t) &= \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} \partial_t\psi_N(v_1;v_2,\ldots,v_N,t)\,d\sigma_1 \\ &= \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_1^2}\right)} K(\psi_N)(v_1,v_2,\ldots,v_N,t)\,d\sigma_1 \ .\end{aligned} \tag{1.17}$$

Evaluating this integral, making use of the symmetry condition on ψ_N, and using the form of f_2^N as defined in Eq. 1.16 gives

$$\partial_t f_1^N(v_1,t) = 2\int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} \frac{1}{2\pi}\int_0^{2\pi}\left(f_2^N(v_1',v_2',t) - f_2^N(v_1,v_2,t)\right)d\theta\,dv_2 \ , \tag{1.18}$$

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 Eq. 1.6. Note that, instead of $f(v,t)\,f(v_*,t)$ as in Eq. 1.7, here we have $f_2^N(v_1,v_2,t)$. Further, Eq. 1.18 is not a closed equation when N is finite.

A key issue in the connection between the dynamics of many-particle systems as governed by the linear model Eq. 1.12 and the Boltzmann equation Eq. 1.6, is the notion of propagation of molecular chaos [21, 28, 23, 25, 10, 22]. It deals with the hypothesis that molecular chaos, i.e. the stochastic independence of two random particles in a many-particle system, persists in time, in the limit of infinitely many particles.

Definition 1.1 (Kac [21] on the Boltzmann property) *Consider the sequence of probability density functions $\psi_N \equiv \psi_N(v_1,\ldots,v_N,0)$ defined on $\mathbb{S}^{N-1}(\sqrt{N})$. This ψ_N 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.

Theorem 1.1 (Kac [21] on the propagation of chaos) *If $\psi_N(v_1, \ldots, v_N, 0)$ has the Boltzmann property, then $\psi_N(v_1, \ldots, v_N, t)$, i.e. the solution of Eq. 1.12, has the Boltzmann property,*

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

This says that the Boltzmann property propagates in time. Moreover, the limit $f_1(v_1, t)$ of the single-particle marginal $f_1^N(v_1, t)$ satisfies Eq. 1.6.

A particular case is $k = 2$, which results in

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

which in turn is used in recovering Eq. 1.7 from Eq. 1.18.

A simple, but illuminating example is to consider the sequence of probability distributions consisting of the constant function, the distribution ψ_N given by

$$\psi_N(\mathbf{V}, t) \ = \ \frac{1}{\left|S^{N-1}(\sqrt{N})\right|} \ , \tag{1.19}$$

where $\left|S^{N-1}(\sqrt{N})\right|$ denotes the surface measure of $S^{N-1}(\sqrt{N})$. The single-particle marginal corresponding to this ψ_N is

$$f_1^N(v_1) \ = \ \frac{\left(1 - \frac{v_1^2}{N}\right)^{\frac{N-3}{2}}}{\int_{-\sqrt{N}}^{\sqrt{N}} \left(1 - \frac{v_1^2}{N}\right)^{\frac{N-3}{2}} dv} \ , \tag{1.20}$$

which, in the limit $N \to \infty$, becomes the Maxwellian density

$$M(v_1) \ = \ \frac{1}{\sqrt{2\pi}} e^{-\frac{v_1^2}{2}} \ . \tag{1.21}$$

We note that, the constant function given in Eq. 1.19 is the unique stationary state of Eq. 1.12, and the Maxwellian distribution M is the stationary state of Eq. 1.6.

Chapter 2

Kac's Master Equation with a Gaussian Thermostat

2.1 The Thermostated System

The original Kac dynamics, as described by the master equation Eq. 1.12, is all due to the random jumps which correspond to the random collisions. It is also interesting to incorporate, in addition to the collisions, a driving force field into the system. This has been studied in connection with the Lorentz model for conduction in metals. Detailed numerical and analytical studies 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 made in [8, 9, 26].

We consider a Kac system of N point particles, with an external uniform force field $\mathbf{E} \in \mathbb{R}^N$, such that $|\mathbf{E}| = E$. The motion of the point $\mathbf{V} \in \mathbb{R}^N$ is governed by the equation $\frac{d\mathbf{V}}{dt} = \mathbf{E}$. This results in energy being supplied into the system, and drives the system away from equilibrium. To eliminate this excess energy we introduce a thermostat - a term which forces the dynamics to keep the total kinetic energy constant. This is accomplished by replacing the above dynamics with

$$\frac{d\mathbf{V}}{dt} = \mathbf{E} - T(\mathbf{V}) \ , \tag{2.1}$$

where $T(\mathbf{V})$ represents the effect of the thermostat, which keeps $\mathbf{V}$ on the energy surface $\Sigma \equiv \{\mathbf{V} \in \mathbb{R}^N : |\mathbf{V}|^2 = C\}$, for some positive constant C. With such a thermostat, Eq. 2.1 becomes

$$\frac{d\mathbf{V}}{dt} = \mathbf{E} - \frac{\mathbf{E}\cdot\mathbf{V}}{|\mathbf{V}|^2}\mathbf{V} \ . \tag{2.2}$$

This is just constraining the evolution governed by $\frac{d\mathbf{V}}{dt} = \mathbf{E}$ to Σ, by projecting the field $\mathbf{E}$ onto the tangent plane to Σ at $\mathbf{V}$. This gives what is known as a Gaussian iso-kinetic thermostat [14, 16, 18, 27, 26].

By introducing the quantities $J \equiv J(t)$ and $U \equiv U(t)$ as

$$J = \frac{1}{N}\sum_{i=1}^{N} v_i(t) \qquad \text{and} \qquad U = \frac{1}{N}\sum_{i=1}^{N} v_i(t)^2 \ , \tag{2.3}$$

and recalling that $|\mathbf{E}| = E$, Eq. 2.2 can be rewritten as

$$\frac{d\mathbf{V}}{dt} \ = \ \mathbf{E} - \frac{J}{U}\mathbf{E}\cdot\mathbf{V}, \tag{2.4}$$

or component-wise as

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

where $\mathbf{E} = E\,(1,1,\ldots,1)^t \in \mathbb{R}^N$, and J satisfies the equation

$$\frac{dJ(t)}{dt} \ = \ E - \frac{E}{U}J(t)^2 \ . \tag{2.6}$$

On the other hand,

$$\begin{aligned} \frac{dU(t)}{dt} \ &= \ \frac{2}{N}\sum_{i=1}^{N} v_i(t)\,\frac{dv_i(t)}{dt} \\ &= \ \frac{2\,E}{N}\sum_{i=1}^{N}\Big(v_i(t) \ - \ \frac{J}{U}\,v_i(t)\Big) \ = \ 0 \ , \end{aligned}$$

which implies that U is constant in time.

Given an initial data $J(t_0) = J_0$, Eq. 2.6 can be solved exactly to give

$$J(t) = \frac{J_0\cosh(\frac{E}{\sqrt{U}}t) + \sqrt{U}\sinh(\frac{E}{\sqrt{U}}t)}{\frac{J_0}{\sqrt{U}}\sinh(\frac{E}{\sqrt{U}}t) + \cosh(\frac{E}{\sqrt{U}}t)} \ . \tag{2.7}$$

It is then possible to rewrite Eq. 2.4 as

$$\frac{dv_i(t)}{dt} + \frac{E}{U}J(t)v_i(t) \ = \ E \ , \qquad i = 1,2,3,\ldots,N \tag{2.8}$$

and solve it, with an initial data $v_i(t_0)$, to get

$$v_i(t) = \frac{\sqrt{U}\sinh(\frac{E}{\sqrt{U}}t) + J_0\cosh(\frac{E}{\sqrt{U}}t) - J_0 + v_i(t_0)}{\cosh(\frac{E}{\sqrt{U}}t) + \frac{J_0}{\sqrt{U}}\sinh(\frac{E}{\sqrt{U}}t)} \ , \quad i = 1,2,3,\ldots,N \ . \tag{2.9}$$

This describes the velocity of each particle before any possible subsequent collision. Note that, as $t \to \infty$, all the v_i converge to $\sqrt{U}$:

$$v_i(t) \to \sqrt{U} \quad \text{as } t \to \infty \ . \tag{2.10}$$

2.2 The Master Equation and the Resulting Boltzmann Equation

Let $\psi_N \equiv \psi_N(\mathbf{V},t)$ be the probability density of the N velocities at time t, i.e. for each $t \geq 0$, $\psi_N \geq 0$ is a real-valued function defined on $\mathbb{S}^{N-1}(\sqrt{N})$, and such that

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} \psi_N(\mathbf{V},t)\, d\sigma_0 \;=\; 1 \;.$$

Further, for a region $A \subset \mathbb{S}^{N-1}\big(\sqrt{N}\big)$, the probability that $\mathbf{V}$ is in A at time t is given by

$$P(\mathbf{V} \in A) \;=\; \int_A \psi_N(\mathbf{V},t)\, d\sigma_0 \;.$$

The unique solution to Eq. 2.2 with initial data $\mathbf{V}_0$ defines an evolution operator T^t such that $\mathbf{V} = T^t\mathbf{V}_0$. We further note that, for a fixed t, $\mathbf{V}$ is a function of $\mathbf{V}_0$, and if we denote the Jacobian determinant by $\mathcal{J}$, we get the condition that $\partial_t\big(\psi_N(\mathbf{V}(t,\mathbf{V}_0),t)\ \mathcal{J}\big) \;=\; 0$, which in turn, since $\mathcal{J} \neq 0$, results in

$$\frac{\partial \psi_N}{\partial t} \;+\; \nabla\psi_N \cdot \frac{d\mathbf{V}}{dt} \;+\; \psi_N \frac{1}{\mathcal{J}}\frac{\partial \mathcal{J}}{\partial t} \;=\; 0 \;. \tag{2.11}$$

To explore the coupling to Eq. 2.4, we denote the vector field

$$\tilde{\mathbf{F}} \;\equiv\; \tilde{\mathbf{F}}(\mathbf{V}) \;=\; \mathbf{E} - \frac{J}{U}\,\mathbf{E}\cdot\mathbf{V} \;, \tag{2.12}$$

where J and U are as specified in Eq. 2.3, and $\mathbf{E} \in \mathbb{R}^N$ is the applied field. Then we can rewrite Eq. 2.11 as

$$\frac{\partial \psi_N}{\partial t} \;+\; \nabla\psi_N \cdot \tilde{\mathbf{F}} \;+\; \psi_N\, \nabla\cdot\tilde{\mathbf{F}} \;=\; 0 \;, \tag{2.13}$$

which takes the form of the continuity equation

$$\frac{\partial \psi_N}{\partial t} \;+\; \nabla\cdot\big(\tilde{\mathbf{F}}\,\psi_N\big) \;=\; 0 \;. \tag{2.14}$$

Eq. 2.14 says that, the number of particles is conserved.

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

$$\mathbf{F} \;\equiv\; N\sqrt{U}\;\nabla\Big(\frac{J}{\sqrt{U}}\Big) \;=\; \Big(1 - \frac{J}{U}v_1, \ldots, 1 - \frac{J}{U}v_N\Big) \;. \tag{2.15}$$

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

Up until now the dynamics was due only to the driving field $\tilde{\mathbf{F}}$. If we further allow collisions to occur then the distribution function ψ_N will evolve in time according to the equation

$$\frac{\partial \psi_N}{\partial t} \;+\; E\,\nabla\cdot\big(\mathbf{F}\ \psi_N\big) \;=\; K(\psi_N) \;, \tag{2.16}$$

where $\mathbf{F}$ is as in Eq. 2.15, and K is as defined in Eq. 1.13. This forms the Kac-like master equation upon which our studies and results are based.

Theorem 2.1 *Suppose that $\psi_N \equiv \psi_N(v_1,\ldots,v_N,t)$ is a sequence of C^1-solutions to Eq. 2.16 and that ψ_N is symmetric in the variables $v_1,\ldots,v_N$. If ψ_N has the Boltzmann property, and if further*

$$f(v,t) \;=\; \lim_{N\to\infty} f_1^N(v_1,t),$$

exists, then $f \equiv f(v,t)$ satisfies the Boltzmann equation

$$\partial_t f \;+\; E\,\partial_v\Big(\big(1-\zeta\,v\big)\,f\Big) \;=\; Q(f,f), \tag{2.17}$$

where $\zeta \equiv \zeta(t)$ is given by

$$\zeta \;=\; \int_{-\infty}^{\infty} v\,f(v,t)\,dv\ , \tag{2.18}$$

and $Q(f,f)$ is as given in Eq. 1.7.

Notation : In the sequel, for the sake of simplicity, we denote the surface $\mathbb{S}^{N-1}\big(\sqrt{N}\big)$ 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: Consider the single-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 Eq. 1.14 ,

$$f_1^N(v_1,t) \;=\; \int_{\Omega_1} \psi_N(v_1;v_2,\ldots,v_N,t)\;d\sigma_1\ , \tag{2.19}$$

$$f_2^N(v_1,v_2,t) \;=\; \int_{\Omega_2} \psi_N(v_1,v_2;v_3,\ldots,v_N,t)\;d\sigma_2\ . \tag{2.20}$$

Differentiating $f_1^N(v_1,t)$ with respect to t and using Eq. 2.16 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

$$\frac{\partial}{\partial t} f_1^N(v_1,t) + E\int_{\Omega_1} \nabla\cdot\big(\mathbf{F}\;\psi_N\big)\;d\sigma_1 \;=\; \int_{\Omega_1} K(\psi_N)\;d\sigma_1\ . \tag{2.21}$$

We recall Kac's result in section 1.2 that, in the limit $N\to\infty$, the integral $\displaystyle\int_{\Omega_1} K(\psi_N)\;d\sigma_1$ takes the form $Q(f,f)$ as given in Eq. 1.7. The rest of the proof then follows through the result of Proposition 2.1. ■

Proposition 2.1 *Let the densities $\psi_N(v_1,\ldots,v_N,t)$ be as specified in Theorem 2.1, let ζ be as defined in Eq. 2.18, and let* $\mathbf{F}$ *be as given in Eq. 2.15. Then, in the limit $N\to\infty$, we have that*

$$\int_{\Omega_1} \nabla\cdot\big(\mathbf{F}\ \psi_N\big)\ d\sigma_1 \quad\longrightarrow\quad \partial_v\Big((1-\zeta v)f\Big)\ . \tag{2.22}$$

Proof : Let $\phi\in C_0^1(\mathbb{R})$ be such that $\phi=\phi(v_1)$, 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 that $\nabla\eta_r\cdot\mathbf{F}=0$, where ∇ denotes $\nabla_{\mathbf{V}}$. Further we have that $\nabla\phi\cdot\mathbf{F}\ =\ N\big(\partial_{v_1}\phi\big)\big(1-\frac{J}{U}v_1\big)$.

We start by noting that,

$$\int_{\Omega_0}\phi\ \nabla\cdot(\mathbf{F}\ \psi_N)\ d\sigma_0=\int_{-\sqrt{N}}^{\sqrt{N}}\phi\ \left\{\sqrt{\frac{N}{N-v_1^2}}\ \int_{\Omega_1}\nabla\cdot(\mathbf{F}\ \psi_N)\,d\sigma_1\right\}dv_1\ .$$

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

$$\int_{\Omega_0}\phi\ \nabla\cdot(\mathbf{F}\ \psi_N)\ d\sigma_0=\frac{d}{dr}\Big(\int_{\mathbb{R}^N}\eta_r\ \phi\ \nabla\cdot(\mathbf{F}\ \psi_N)\,d\mathbf{V}\Big)\Big|_{r=\sqrt{N}}\ .$$

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. Now integration by parts gives

$$\begin{aligned}\int_{\mathbb{R}^N}\eta_r\ \phi\ \nabla\cdot(\mathbf{F}\ \psi_N)\,d\mathbf{V}\ &=\ -\int_{\mathbb{R}^N}\nabla\big(\eta_r\ \phi\big)\cdot(\mathbf{F}\ \psi_N)\,d\mathbf{V}\\ &=\ -\int_{\mathbb{R}^N}\phi\ \nabla\eta_r\cdot(\mathbf{F}\ \psi_N)\,d\mathbf{V}-\int_{\mathbb{R}^N}\eta_r\nabla\phi\cdot(\mathbf{F}\ \psi_N)\,d\mathbf{V}\\ &=\ -\int_{\mathbb{R}^N}\eta_r\ \Big(\partial_{v_1}\phi\Big)\Big(1-\frac{J}{U}v_1\Big)\,\psi_N\,d\mathbf{V}\\ &=\ -\int_{-\infty}^{\infty}\Big(\partial_{v_1}\phi\Big)\Big\{\int_{\mathbb{R}^{N-1}}\eta_r\ \Big(1-\frac{J}{U}\ v_1\Big)\ \psi_N\ dv_2\cdots dv_N\Big\}\ dv_1\ .\end{aligned}$$

Here we have made use of both the fact that $\nabla\eta_r\cdot\mathbf{F}=0$ and that $\phi=\phi(v_1)$. Then the above integral equals

$$-\int_{-\infty}^{\infty}\Big(\partial_{v_1}\phi\Big)\Big\{\int_0^{\sqrt{r^2-v_1^2}}\Big(\int_{\mathbb{S}^{N-2}(\sqrt{r^2-v_1^2})}\Big(1-\frac{J}{U}\,v_1\Big)\,\psi_N\,d\sigma_2\Big)\,dr\Big\}\,dv_1\ ,$$

and writing $\rho\boldsymbol{w}=(v_2,\ldots,v_N)$, with $\boldsymbol{w}\in\mathbb{S}^{N-2}$ and $\rho>0$, gives

$$-\int_{-\infty}^{\infty}\Big(\partial_{v_1}\phi\Big)\Big\{\int_0^{\sqrt{r^2-v_1^2}}\int_{\mathbb{S}^{N-2}}\Big(1-\frac{v_1+\rho\boldsymbol{w}}{v_1^2+\rho^2}v_1\Big)\psi_N(v_1;\rho\boldsymbol{w})\,\rho^{N-2}\,d\boldsymbol{w}\,d\rho\Big\}dv_1\ . \tag{2.23}$$

Differentiating the inner term with respect to r we see that

$$\begin{aligned} &\frac{d}{dr}\left[\int_0^{\sqrt{r^2-v_1^2}} \int_{\mathbb{S}^{N-2}} \Big(1-\frac{v_1+\rho\boldsymbol{w}}{v_1^2+\rho^2}\,v_1\Big)\,\psi_N\,\rho^{N-2}\,d\boldsymbol{w}\,d\rho\right] \\ &\qquad = \frac{r}{\sqrt{r^2-v_1^2}}\int_{\mathbb{S}^{N-2}}\Big(1-\frac{v_1+\sqrt{r^2-v_1^2}\boldsymbol{w}}{v_1^2+r^2-v_1^2}v_1\Big)\,(r^2-v_1^2)^{\frac{N-2}{2}}\,\psi_N\,d\boldsymbol{w}\ . \end{aligned} \tag{2.24}$$

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

$$\begin{aligned} &\frac{\sqrt{N}}{\sqrt{N-v_1^2}}\int_{\mathbb{S}^{N-2}}\Big(1-\frac{v_1+\sqrt{N-v_1^2}\boldsymbol{w}}{N}v_1\Big)(N-v_1^2)^{\frac{N-2}{2}}\,\psi_N\,d\boldsymbol{w} \\ &\qquad = \frac{\sqrt{N}}{\sqrt{N-v_1^2}}\int_{\Omega_1}\Big(1-\frac{J}{U}v_1\Big)\,\psi_N\,d\sigma_1\ . \end{aligned} \tag{2.25}$$

With proposition 2.2 below, in the limit $N\to\infty$, Eq. 2.23 takes the form

$$-\int_{-\infty}^{\infty}(\partial_{v_1}\phi)\Big((1-\zeta v_1)f\Big)\,dv_1 \;=\; \int_{-\infty}^{\infty}\phi\,\partial_{v_1}\Big((1-\zeta v_1)f\Big)\,dv_1\ . \tag{2.26}$$

Thus we conclude that, as $N\to\infty$,

$$\int_{\Omega_1}\nabla\cdot\big(\mathbf{F}\,\psi_N\big)\,d\sigma_1 \;\longrightarrow\; \partial_v\Big((1-\zeta\,v)\,f\Big)\ . \tag{2.27}$$

■

Proposition 2.2 *Let the densities $\psi_N(v_1,\ldots,v_N,t)$ be as specified in Theorem 2.1 and let ζ be as defined in Eq. 2.18. Then, in the limit $N\to\infty$, we have that*

$$\int_{\Omega_1}\Big(1-\frac{J}{U}\,v_1\Big)\,\psi_N\,d\sigma_1 \quad\longrightarrow\quad (1-\zeta\,v_1)\,f\ . \tag{2.28}$$

Proof: We start by noting that

$$\begin{aligned} \int_{\Omega_1}\Big(1-\frac{J}{U}v_1\Big)\,\psi_N\,d\sigma_1 &= \int_{\Omega_1}\psi_N\,d\sigma_1 - v_1\int_{\Omega_1}\frac{J}{U}\,\psi_N\,d\sigma_1 \\ &= f_1^N(v_1)-v_1\int_{\Omega_1}\frac{J}{U}\,\psi_N\,d\sigma_1\ . \end{aligned} \tag{2.29}$$

We then use the form of J and the symmetry condition on ψ_N to get

$$\begin{aligned} \int_{\Omega_1}\frac{J}{U}\,\psi_N\,d\sigma_1 &= \int_{\Omega_1}\frac{v_1}{U}\,\psi_N\,d\sigma_1+\int_{\Omega_1}\frac{v_2+\cdots+v_N}{U}\,\psi_N\,d\sigma_1 \\ &= \frac{1}{N}\,v_1\,f_1^N \;+\; \frac{N-1}{N}\int_{\Omega_1}v_2\,\psi_N\,d\sigma_1\ . \end{aligned} \tag{2.30}$$

By writing the integral in Eq. 2.30 as an iterated integral, and using the expression in Eq. 2.25 adapted to Ω_2 gives

$$\begin{aligned} \int_{\Omega_1}v_2\,\psi_N\,d\sigma_1 &= \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\left\{\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\int_{\Omega_2}\psi_N(v_1,v_2;v_3,\ldots,v_N,t)\,d\sigma_2\right\}dv_2 \\ &= \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\,\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\;f_2^N(v_1,v_2,t)\,dv_2\ . \end{aligned} \tag{2.31}$$

By assumption ψ_N has the Boltzmann property, and hence

$$f_2^N(v_1,v_2,t) \;\longrightarrow\; f(v_1,t)\,f(v_2,t) \qquad \text{as } N\to\infty$$

and hence the above integral (Eq. 2.31) equals

$$\begin{aligned}&\int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2\, f_1^N(v_1,t)\, f_1^N(v_2,t)\, dv_2 \\ &\qquad + \int_{-\sqrt{N-v_1^2}}^{\sqrt{N-v_1^2}} v_2 \left[\sqrt{\frac{N-v_1^2}{N-v_1^2-v_2^2}}\; f_2^N(v_1,v_2,t) - f_1^N(v_1,t)\, f_1^N(v_2,t)\right] dv_2\ .\end{aligned} \tag{2.32}$$

Because of our assumption, the functions f_k^N decay sufficiently fast that passing to the limit ($N\to\infty$), the terms in Eq. 2.31 converge to $f(v,t)\int_{-\infty}^{\infty} v\, f(v,t)\, dv$.

By combining Eq. 2.31, Eq. 2.30, and Eq. 2.29; letting $N\to\infty$, we conclude that

$$\int_{\Omega_1}\left(1-\frac{J}{U}v_1\right)\psi_N\; d\sigma_1 \;\longrightarrow\; (1-\zeta v_1) f\ .$$

■

2.3 Stationary States

In this section we consider the stationary case of Eq. 2.17, and present an expression for the steady current ζ as a function of the force field. We also prove existence of a stationary state solution to Eq. 2.17 in a particular case.

The stationary case of Eq. 2.17 is

$$E\,\frac{d}{dv}\Big((1-\zeta\, v)\, f(v)\Big) \;=\; Q(f,f)(v), \tag{2.33}$$

where the steady current ζ is given by

$$\zeta \;=\; \int_{-\infty}^{\infty} v\, f(v)\, dv, \tag{2.34}$$

and

$$Q(f,f)(v) \;=\; \int_{-\infty}^{+\infty}\int_0^{2\pi}\Big(f(v')\, f(v'_*) \;-\; f(v)\, f(v_*)\Big)\,\frac{1}{2\pi}\, d\theta\, dv_*, \tag{2.35}$$

with v' and v'_* as given in Eq. 1.8.

Corresponding to the result in Eq. 1.5, we note that, for sufficiently regular function $\phi\equiv\phi(v)$, the collision integral Q in Eq. 2.35 fulfils

$$\int_{-\infty}^{+\infty}\phi(v)\, Q(f,f)(v)\, dv \;=\; \frac{1}{2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi}\left(\phi'_*+\phi'-\phi_*-\phi\right) f\, f_*\,\frac{1}{2\pi}\, d\theta\, dv_*\, dv\ . \tag{2.36}$$

Proposition 2.3 *Consider ζ as defined in Eq. 2.34. Assume that there exist a non-negative solution f to Eq. 2.33 such that $\int_{-\infty}^{+\infty} f(v)\,dv = 1$, and $v^2 f(v) \to 0$ as $|v| \to \infty$. Then the steady current ζ is*

$$\zeta \;=\; \frac{2E}{\sqrt{1+4E^2}+1}\;. \tag{2.37}$$

Proof : Multiplying both sides of Eq. 2.33 by v, integrating the resulting equation with respect to v, using Eq. 2.36 with $\phi(v) = v$, and noting that $\int_0^{2\pi} v'\,d\theta = 0$, gives

$$\begin{aligned}
\frac{1}{E}\int_{-\infty}^{+\infty} v\,Q(f,f)\,dv &= \frac{1}{E}\,\frac{1}{2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} f(v_*)\,f(v)\big[v'_* + v' - v_* - v\big]\frac{1}{2\pi}\,d\theta\,dv_*\,dv \\
&= -\frac{1}{2E}\,\frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} f(v_*)f(v)\big[v_* + v\big]d\theta\,dv_*\,dv \\
&= -\frac{1}{E}\,\zeta\;.
\end{aligned}\tag{2.38}$$

On the other hand, by partial integration

$$\begin{aligned}
\int_{-\infty}^{+\infty} v\,\frac{d}{dv}\Big((1-\zeta\,v)\,f(v)\Big)\,dv &= -\int_{-\infty}^{+\infty}(1-\zeta\,v)\,f(v)\,dv \\
&= -1 \;+\; \zeta^2\;.
\end{aligned}\tag{2.39}$$

Equating Eq. 2.38 and Eq. 2.39 leads to the following quadratic equation in ζ,

$$\zeta^2 \;+\; \frac{1}{E}\,\zeta \;-\; 1 \;=\; 0\;,$$

whose roots are $\zeta_{1,2} = \dfrac{-1 \pm \sqrt{1+4E^2}}{2E}$.

We then note, using Hölder's inequality, that $\big|\int_{-\infty}^{+\infty} v\,f(v)\,dv\big| \le 1$. But since $\big|\frac{-1-\sqrt{1+4E^2}}{2E}\big| > 1$, we conclude that

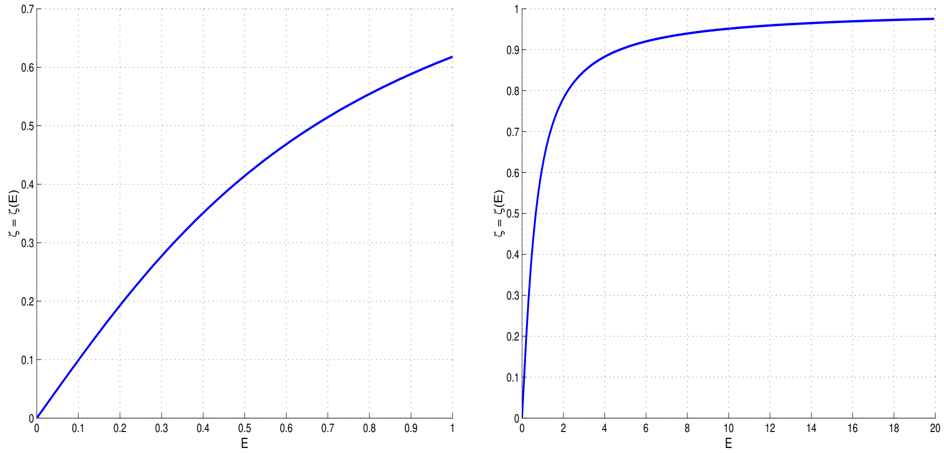
$$\zeta \;\equiv\; \zeta(E) \;=\; \frac{2E}{\sqrt{1+4E^2}+1}\;. \tag{2.40}$$

This completes the proof. ■

We see that, in the limit $E \to 0$ we have $\zeta \to 0$. This behaviour of ζ is depicted in Figure 2.1a for relatively small values of the force field E. Further, in the limit $E \to \infty$ we have that $\zeta \to 1$. This trend is also indicated in Figure 2.1b for relatively big values of E.

Towards stating and proving the existence of a stationary solution, we consider and reformulate Eq. 2.33. When $\int_{-\infty}^{+\infty} f(v)\,dv = 1$, the collision integral Q given in Eq. 2.35 can be rewritten as

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



a. b.

Figure 2.1: Steady current ζ as a function of E.

where

$$Q^+(f,f)(v) \;=\; \int_{-\infty}^{+\infty}\int_0^{2\pi} f(v')\, f(v'_*)\, \frac{1}{2\pi}\, d\theta\, dv_* \ .$$

Using this form of Q in Eq. 2.33 results in

$$\big(\frac{1}{E}-\zeta\big)\, f + \big(1-\zeta\, v\big)\, \frac{d}{dv} f \;=\; \frac{1}{E}\, Q^+(f,f)\ . \tag{2.41}$$

The case $\zeta = \dfrac{1}{E}$, on the one hand transforms Eq. 2.41 to

$$\big(1-\zeta\, v\big)\, \frac{d}{dv} f \;=\; \frac{1}{E}\, Q^+(f,f)\ . \tag{2.42}$$

But $\zeta = \dfrac{1}{E}$ also means that

$$\frac{2E}{\sqrt{1+4E^2}+1} \;=\; \frac{1}{E}\ ,$$

and this holds only if $E=\sqrt{2}$, since $E>0$.

Theorem 2.2 *Let $E=\sqrt{2}$. Then Eq. 2.33 has a non-negative solution f which is continuous except at $v=\sqrt{2}$.*

Proof : The value $E=\sqrt{2}$ transforms Eq. 2.42 to

$$\frac{d}{dv} f(v) \;=\; \frac{1}{\sqrt{2}-v}\; Q^+(f,f)(v)\ . \tag{2.43}$$

The existence result is established through iteration. Having choosen $f_1(v)\geq 0$ such that $\displaystyle\int_{-\infty}^{+\infty} f_1(v)\, dv = 1$, we introduce the iteration

$$f_{n+1}(v) \;=\; \mathcal{A}(f_n)(v)\ , \qquad \text{for} \quad n=1,\,2,\,3,\,\ldots \tag{2.44}$$

where $\mathcal{A}$ is given by

$$\mathcal{A}(f)(v) \;=\; \begin{cases} \displaystyle\int_{-\infty}^{v} \frac{1}{\sqrt{2}-w}\, Q^{+}(f,f)(w)\, dw \;, & \text{for } \; v<\sqrt{2} \\[2ex] \displaystyle\int_{v}^{+\infty} \frac{1}{w-\sqrt{2}}\, Q^{+}(f,f)(w)\, dw \;, & \text{for } \; v>\sqrt{2} \;. \end{cases}$$

From this very definition of $\mathcal{A}$ we see that $f_n \geq 0$, for every n, and it is also easy to see that $\mathcal{A}(f)(v) \;\leq\; \dfrac{1}{|v-\sqrt{2}|}$.

Multiplying both sides of Eq. 2.44 by a continuous and bounded function $\phi \equiv \phi(v)$, and integrating with respect to v, gives

$$\int_{-\infty}^{+\infty} \phi(v)\, f_{n+1}(v)\, dv \;=\; \int_{-\infty}^{+\infty} \phi(v)\, \mathcal{A}(f_n)(v)\, dv \;, \tag{2.46}$$

for $n = 1, 2, 3, \ldots$.

To put the right hand side of Eq. 2.46 in a more convenient form, we write

$$\begin{aligned} \int_{-\infty}^{+\infty} \phi(v)\, \mathcal{A}(f)(v)\, dv \;&=\; \int_{-\infty}^{\sqrt{2}} \phi(v) \left\{ \int_{-\infty}^{v} \frac{1}{\sqrt{2}-w}\, Q^{+}(f,f)(w)\, dw \right\} dv \\ &\quad + \int_{\sqrt{2}}^{+\infty} \phi(v) \left\{ \int_{v}^{+\infty} \frac{1}{w-\sqrt{2}}\, Q^{+}(f,f)(w)\, dw \right\} dv \\ &=\; \int_{-\infty}^{\sqrt{2}} \left(\int_{w}^{\sqrt{2}} \phi(v)\, dv \right) \frac{1}{\sqrt{2}-w}\; Q^{+}(f,f)(w)\, dw \\ &\quad + \int_{\sqrt{2}}^{+\infty} \left(\int_{\sqrt{2}}^{w} \phi(v)\, dv \right) \frac{1}{w-\sqrt{2}}\; Q^{+}(f,f)(w)\, dw \\ &=\; \int_{-\infty}^{+\infty} \frac{1}{w-\sqrt{2}} \left(\int_{\sqrt{2}}^{w} \phi(v)\, dv \right) Q^{+}(f,f)(w)\, dw \;. \end{aligned} \tag{2.47}$$

Let

$$\Phi(v) \;=\; \frac{1}{v-\sqrt{2}} \int_{\sqrt{2}}^{v} \phi(z)\, dz \;, \tag{2.48}$$

and rewrite Eq. 2.47 as

$$\int_{-\infty}^{+\infty} \phi(v)\, \mathcal{A}(f)(v)\, dv \;=\; \int_{-\infty}^{+\infty} \Phi(v)\, Q^{+}(f,f)(v)\, dv \;. \tag{2.49}$$

Using the transformation used in Eq. 2.36

$$\int_{-\infty}^{+\infty} \phi(v)\, \mathcal{A}(f)(v)\, dv \;=\; \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(v) f(v_*) \left(\frac{1}{2\pi} \int_{0}^{2\pi} \frac{\int_{\sqrt{2}}^{v'} \phi(z)\, dz}{v'-\sqrt{2}}\, d\theta \right) dv_*\, dv \;. \tag{2.50}$$

Letting

$$\Psi \;\equiv\; \Psi(v, v_*) \;=\; \frac{1}{2\pi}\int_0^{2\pi} \frac{\int_{\sqrt{2}}^{v'} \phi(z)\,dz}{v' - \sqrt{2}}\,d\theta \;, \tag{2.51}$$

Eq. 2.50 can be written as

$$\int_{-\infty}^{+\infty} \phi(v)\,\mathcal{A}(f)(v)\,dv \;=\; \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Psi(v, v_*)\,f(v)\,f(v_*)\,dv\,dv_* \;. \tag{2.52}$$

We also note that, Ψ is uniformly continuous in v and v_*, and it is bounded.

To study the moments, let $\phi(v) = v^k$ for $k = 0, 1, 2, \ldots$, so that Φ takes the form

$$\begin{aligned}\Phi(v) \;&=\; \frac{1}{k+1}\,\frac{v^{k+1} - \sqrt{2}^{k+1}}{v - \sqrt{2}}\\[1em] &=\; \frac{1}{k+1}\,\sum_{j=0}^{k} v^j\,\sqrt{2}^{k-j} \;.\end{aligned}$$

We recall $v' = v\cos\theta + v_*\sin\theta$. This implies that, for all odd k,

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} {v'}^k\,f(v)\,f(v_*)\,\frac{1}{2\pi}\,d\theta\,dv_*\,dv \;=\; 0 \;. \tag{2.53}$$

Further, for a continuous function g, change of variables gives that,

$$\begin{aligned}&\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} g(v)\,f(v')\,f(v_*')\,\frac{1}{2\pi}\,d\theta\,dv_*\,dv\\ &\qquad\qquad = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} g(v')\,f(v)\,f(v_*)\,\frac{1}{2\pi}\,d\theta\,dv_*\,dv \;.\end{aligned} \tag{2.54}$$

For $k = 0$, or $\phi(v) = 1$, we have that $\Phi(v) = 1$. Put into Eq. 2.50, this gives

$$\begin{aligned}\int_{-\infty}^{+\infty} \mathcal{A}(f)(v)\,dv \;&=\; \int_{-\infty}^{+\infty} Q^+(f,f)(v)\,dv\\[1em] &=\; \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} f(v)\,f(v_*)\,\frac{1}{2\pi}\,d\theta\,dv_*\,dv\\[1em] &=\; \left[\int_{-\infty}^{+\infty} f(v)\,dv\right]^2.\end{aligned}$$

This, with Eq. 2.46, says that, $\displaystyle\int_{-\infty}^{+\infty} f_{n+1}(v)\,dv = \Big(\int_{-\infty}^{+\infty} f_n(v)\,dv\Big)^2$. This verifies that, in the iteration Eq. 2.44, $\displaystyle\int_{-\infty}^{+\infty} f_n(v)\,dv = 1$, for every n, if $\displaystyle\int_{-\infty}^{+\infty} f_1(v)\,dv = 1$.

For $\phi(v) = v$, we get $\Phi(v) = \frac{1}{2}(v + \sqrt{2})$, so that from Eq. 2.50 again

$$\begin{aligned}\int_{-\infty}^{+\infty} v\,\mathcal{A}(f)(v)\,dv \;&=\; \frac{1}{2}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{2\pi} \Big(v' + \sqrt{2}\Big)\,f(v)\,f(v_*)\,\frac{1}{2\pi}\,d\theta\,dv_*\,dv\\[1em] &=\; \frac{1}{\sqrt{2}}\Big(\int_{-\infty}^{+\infty} f(v)\,dv\Big)^2 \;.\end{aligned}$$

Using this with Eq. 2.46, we have

$$\int_{-\infty}^{+\infty} v\, f_{n+1}(v)\, dv \;=\; \frac{1}{\sqrt{2}} \Big[\int_{-\infty}^{+\infty} f_n(v)\, dv \Big]^2 \; .$$

But since $\displaystyle\int_{-\infty}^{+\infty} f_n(v)\, dv = 1$, for every n, the result above verifies that, in the iteration Eq. 2.44, $\displaystyle\int_{-\infty}^{+\infty} v\, f_n(v)\, dv = \frac{1}{\sqrt{2}}$, for every n.

Similarly, for $\phi(v) = v^2$, we have $\Phi(v) = v^2 + \sqrt{2}\, v + 2$, so that

$$\begin{aligned}
\int_{-\infty}^{+\infty} v^2\, \mathcal{A}(f)(v)\, dv \;&=\; \frac{1}{3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} \Big(v^2 + \sqrt{2}\, v + 2 \Big) f(v')\, f(v'_*)\, \frac{1}{2\pi}\, d\theta\, dv_*\, dv \\
&=\; \frac{1}{3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} \big(v'^2 + 2 \big) f(v)\, f(v_*)\, \frac{1}{2\pi}\, d\theta\, dv_*\, dv \; . \qquad (2.55)
\end{aligned}$$

Because $v'^2 = v^2 \cos^2\theta + 2v\, v_* \cos\theta \sin\theta + v_*^2 \sin^2\theta$, we have that

$$\begin{aligned}
\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} v'^2 f(v)\, f(v_*)\, \frac{1}{2\pi}\, d\theta\, dv_*\, dv \;&=\; \Big[\int_{-\infty}^{+\infty} v^2\, f(v)\, dv \Big] \Big[\int_{-\infty}^{+\infty} f(v_*)\, dv_* \Big] \\
&=\; \int_{-\infty}^{+\infty} v^2\, f(v)\, dv \; ,
\end{aligned}$$

from which we continue with Eq. 2.55, to get

$$\int_{-\infty}^{+\infty} v^2\, \mathcal{A}(f)(v)\, dv \;=\; \frac{1}{3} \,\Big(\, 2 + \int_{-\infty}^{+\infty} v^2\, f(v)\, dv \Big) \; .$$

Now we use this result in Eq. 2.46, to get

$$\int_{-\infty}^{+\infty} v^2\, f_{n+1}(v)\, dv \;=\; \frac{2}{3} + \frac{1}{3} \int_{-\infty}^{+\infty} v^2\, f_n(v)\, dv \; ,$$

from which we conclude that, $\displaystyle\int_{-\infty}^{+\infty} v^2\, f_n(v)\, dv = 1$, for every n.

With $\phi(v) = v^4$, we have that $\Phi(v) = \frac{1}{5}\big(v^4 + \sqrt{2}\, v^3 + 2v^2 + 2\sqrt{2}\, v + 4 \big)$, so that

$$\begin{aligned}
\int_{-\infty}^{+\infty} v^4\, \mathcal{A}(f)(v)\, dv \;&=\; \frac{1}{5} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} \Big(v^4 + \sqrt{2}\, v^3 + 2v^2 + 2\sqrt{2}\, v + 4 \Big) \times \\
&\qquad\qquad f(v')\, f(v'_*)\, \frac{1}{2\pi}\, d\theta\, dv_* dv \\
&=\; \frac{1}{5} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} \big(v'^4 + 2v'^2 + 4 \big)\, f(v)\, f(v_*)\, \frac{1}{2\pi}\, d\theta\, dv_* dv \; . \qquad (2.56)
\end{aligned}$$

Evaluating the integrals, we get

$$\begin{aligned}
\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{2\pi} v'^4 f(v) f(v_*) \frac{d\theta}{2\pi} dv_* dv \;&=\; \frac{3}{4} \int_{-\infty}^{+\infty} v^4 f(v) dv + \frac{3}{4} \Big[\int_{-\infty}^{+\infty} v^2 f(v) dv \Big]^2 \\
&=\; \frac{3}{4} \int_{-\infty}^{+\infty} v^4\, f(v)\, dv \;+\; \frac{3}{4} \; ,
\end{aligned}$$

so that
$$\int_{-\infty}^{+\infty} v^4\, \mathcal{A}(f)(v)\, dv \;=\; \frac{27}{20} + \frac{3}{20}\int_{-\infty}^{+\infty} v^4\, f(v)\, dv \;.$$
Using this result in Eq. 2.46, we obtain
$$\int_{-\infty}^{+\infty} v^4\, f_{n+1}(v)\, dv \;=\; \frac{27}{20} + \frac{3}{20}\int_{-\infty}^{+\infty} v^4\, f_n(v)\, dv \;.$$
This leads us to conclude that, in the iteration Eq. 2.44, $\int_{-\infty}^{+\infty} v^4\, f_n(v)\, dv \;\le\; C$, for every n, where C is some non-negative constant. In fact, $\int_{-\infty}^{+\infty} v^4\, f_n(v)\, dv \to \frac{27}{17}$ as $n \to \infty$, and similarily one can compute all moments to the stationary state.

Now, the iteration in Eq. 2.44 gives a family of measures with total mass 1 and finite energy. The finite energy implies that $\int_{|v|>K} f_n(v)\, dv \to 0$ as $K \to \infty$, uniformly in n. The family of normalised measures so constructed is, therefore, relatively compact [3]. The sequence f_n has a weakly convergent subsequence, i.e. there exist a subsequence f_{n_i} and a measure μ such that $f_{n_i} \rightharpoonup \mu$. This subsequence is, from now on, denoted by f_n.

The operator $\mathcal{A}(f_n)$ is well defined for all $f_n \in L^1$. To make sense of $\mathcal{A}(\mu)$, which is a measure, we use the form Eq. 2.50. The right hand side there, is well defined also when $f(v)\, dv$ is replaced by a measure $d\mu$. Thus we define $\mathcal{A}(\mu)$ by the expression
$$\int_{-\infty}^{+\infty} \phi(v)\, d\mathcal{A}(\mu) \;=\; \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Psi(v, v_*)\, d\mu(v)\, d\mu(v_*) \;,$$
where Ψ is as given in Eq. 2.51.

Since Ψ is uniformly continuous in v and v_*, and $f_n \rightharpoonup \mu$, we have that
$$\int_{-\infty}^{+\infty} \Psi(v, v_*)\, f_n(v_*)\, dv_* \longrightarrow \int_{-\infty}^{+\infty} \Psi(v, v_*)\, d\mu(v_*) \;, \tag{2.57}$$
uniformly in v, as $n \to \infty$. Further, let
$$\Psi_1 \equiv \Psi_1(v) = \int_{-\infty}^{+\infty} \Psi(v, v_*)\, d\mu(v_*) \;,$$
and note that, Ψ_1 is a continuous and bounded function, so that
$$\int_{-\infty}^{+\infty} \Psi_1(v)\, f_n(v)\, dv \longrightarrow \int_{-\infty}^{+\infty} \Psi_1(v)\, d\mu(v) \;,$$
as $n \to \infty$.

We then consider the difference
$$\begin{aligned}&\int_{-\infty}^{+\infty} \phi(v)\, \mathcal{A}(f_n)(v)\, dv \;-\; \int_{-\infty}^{+\infty} \phi(v)\, d\mathcal{A}(\mu)\\ &\quad= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Psi(v, v_*)\, f_n(v)\, f_n(v_*)\, dv\, dv_* \;-\; \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Psi(v, v_*)\, d\mu(v)\, d\mu(v_*) \;.\end{aligned}$$

Adding and subtracting $\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\,f_n(v)\,dv$, gives

$$\begin{aligned}
&= \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,f_n(v_*)\,dv_*\right]f_n(v)\,dv \;-\; \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]f_n(v)\,dv \\
&\quad + \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]f_n(v)\,dv \;-\; \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]d\mu(v) \\
&= \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,f_n(v_*)\,dv_* - \int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]f_n(v)\,dv \\
&\quad + \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]f_n(v)\,dv \;-\; \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]d\mu(v)\ ,
\end{aligned}$$

and inserting the definition of Ψ_1 makes the above expression equals

$$\begin{aligned}
&= \int_{-\infty}^{+\infty}\left[\int_{-\infty}^{+\infty}\Psi(v,v_*)\,f_n(v_*)\,dv_* - \int_{-\infty}^{+\infty}\Psi(v,v_*)\,d\mu(v_*)\right]f_n(v)\,dv \\
&\quad + \int_{-\infty}^{+\infty}\Psi_1(v)\,f_n(v)\,dv \;-\; \int_{-\infty}^{+\infty}\Psi_1(v)\,d\mu(v)\ .
\end{aligned}\tag{2.58}$$

Because of the uniform convergence in Eq. 2.57, the first term of Eq. 2.58 goes to 0 as $n\to\infty$, and the last difference vanishes in the limit because Ψ_1 is continuous. This verifies the result that $\mathcal{A}(f_n)\rightharpoonup\mathcal{A}(\mu)$. Therefore, $\mu=\mathcal{A}(\mu)$. This completes the proof. ■

We remark that, the uniform bound $f_n(v)\le\dfrac{1}{|v-\sqrt{2}|}$ implies that μ is actually continuous except for a possible singular part concentrated at $v=\sqrt{2}$. A slightly more careful analysis [31] shows that there is no singular part, and that $d\mu(v)\;=\;f(v)\,dv$, with $f(v)\;\sim\;\log\dfrac{1}{|v-\sqrt{2}|}$ near $v=\sqrt{2}$.

2.4 Solution via Hilbert Expansion for Small Force Fields

Here we consider the effect of a force field $\mathbf{E}$ such that $|\mathbf{E}|=\varepsilon$, where $\varepsilon>0$ is small. We use Hilbert expansion technique to derive a non-equilibrium stationary state solution to Eq. 2.33 for these small force fields.

Having the form of the steady current ζ, as a continuous function of ε given in proposition 2.3, we perform a series expansion of type $\zeta=\sum_{k=1}^{\infty}\zeta_k\,\varepsilon^k$ for small values of ε and get

$$\zeta \;=\; \sum_{k=1}^{\infty}\binom{\frac{1}{2}}{k}2^{2k-1}\varepsilon^{2k-1}\ , \tag{2.59}$$

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

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

We remark that, this expansion is convergent for $\varepsilon < 0.5$.

From Eq. 2.59 we deduce that $\zeta_0 = 0$, and for $k = 1, 2, 3, \ldots$

$$\zeta_k \ = \ \begin{cases} 0 \ , & \text{for } \ k \ \text{ even} \\ \binom{\frac{1}{2}}{k} 2^{2k-1} \ , & \text{for } \ k \ \text{ odd} \ . \end{cases}$$

Now we set an expansion of f in powers of ε for solving the stationary case Eq. 2.33. To this end, suppose that f can be written in the form

$$f \ = \ \sum_{k=0}^{\infty} \varepsilon^k f_k \ . \tag{2.60}$$

Further, we introduce the quantities $e_k = \int_{\mathbb{R}} v^2 f_k \, dv$, 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 $\int_{\mathbb{R}} v^m \, M \, dv = 0$ for all odd m, and $\int_{\mathbb{R}} v^m \, M \, dv > 0$ for all even m, where M denotes the Maxwellian.

Inserting the formal series Eq. 2.60 in to Eq. 2.33 gives

$$\sum_{k=0}^{\infty} \varepsilon^k \Big(\frac{d}{dv} f_k - \sum_{j=0}^{k} \zeta_{k-j} \big(f_j + v \, \frac{d}{dv} f_j \big) \Big) \ = \ \sum_{k=0}^{\infty} \varepsilon^{k-1} Q_k \ , \tag{2.61}$$

where

$$\zeta_k \ = \ \int_{-\infty}^{\infty} v \, f_k(v) \, dv \ , \tag{2.62}$$

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

$$Q_k \ = \ \sum_{j=0}^{k} Q(f_j, f_{k-j}) \ . \tag{2.63}$$

In this sum, we find the bilinear form associated with the operator Q as given in Eq. 2.35,

$$Q(f, g) = \frac{1}{2} \int_{-\infty}^{\infty} \int_0^{2\pi} \big(f'_* g' + f' g'_* - f_* g - f g_* \big) \frac{1}{2\pi} d\theta dv_* \ , \tag{2.64}$$

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

We then match the various orders in ε and obtain equations which can be solved recursively. Accordingly, at the ε^{-1} level, we have that $Q(f_0, f_0) = 0$, which holds only if $f_0 = M$, the Maxwellian.

Rewriting Eq. 2.63 as

$$Q_k \;=\; 2Q(M,f_k) \;+\; \sum_{j=1}^{k-1} Q(f_j,f_{k-j}) \;, \tag{2.65}$$

we note that the linear operator $2Q(M,f_k)$ acts on the unknown f_k, while the remainder can be written as a source term, say MS_{k-1}. It is also common to put $f_k = Mh_k$, with $h_0 = 1$, and to consider the h_k as unknown. Eq. 2.65 can therefore be rewritten as

$$Q_k \;=\; MLh_k \;+\; MS_{k-1} \;, \tag{2.66}$$

where the linearised collision operator L is given by

$$Lh_k \;=\; 2M^{-1}Q(M,Mh_k) \;=\; \int_{-\infty}^{\infty}\int_0^{2\pi} M_*\big(h'_{k*}+h'_k-h_{k*}-h_k\big)\frac{1}{2\pi}d\theta\,dv_* \;. \tag{2.67}$$

From this one can see that

$$Lh_k \;=\; 0 \quad\Longleftrightarrow\quad h_k = a+b\,v^2 \quad \text{for}\;\; a,\; b\in\mathbb{R}\;,$$

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

On the other hand, $S_0 = 0$, and for $k = 2,3,4,\ldots$ we have that

$$S_{k-1} \;=\; M^{-1}\sum_{j=2}^{k} Q(Mh_{j-1},Mh_{k+1-j}) \;. \tag{2.68}$$

Using Eq. 2.64 we can rewrite Eq. 2.68 as

$$\begin{aligned} S_{k-1} \;=\; \frac{1}{2}\sum_{j=2}^{k}\int_{-\infty}^{\infty}\int_0^{2\pi} M_*\Big(&h'_{j-1*}h'_{k+1-j} \;+\; h'_{j-1}h'_{k+1-j*} \\ &-\; h_{j-1*}h_{k+1-j} \;-\; h_{j-1}h_{k+1-j*}\Big)\frac{1}{2\pi}\,d\theta\,dv_* \;. \end{aligned} \tag{2.69}$$

At the ε^k level, for $k = 0,1,2,\ldots$, Eq. 2.61 gives

$$-v\,h_k \;+\; \frac{d}{dv}h_k - \sum_{j=0}^{k}\zeta_{k-j}\Big(h_j \;-\; v^2h_j \;+\; v\,\frac{d}{dv}h_j\Big) \;-\; S_k \;=\; L\,h_{k+1} \;. \tag{2.70}$$

For a fixed non-negative integer m consider $g_m(v) = v^m$, a monomial in v of degree m. According to Eq. 2.67, the action of L on such g_m is

$$\begin{aligned} Lg_m(v) = \int_{-\infty}^{\infty}\int_0^{2\pi} M_*\Bigg\{&\sum_{j=0}^{m}\binom{m}{j}v^{m-j}v_*^j\Big((-1)^{m-j}\sin^{m-j}\theta\cos^j\theta+\cos^{m-j}\theta\sin^j\theta\Big) \\ &-\; v_*^m \;-\; v^m\Bigg\}\frac{1}{2\pi}\,d\theta\,dv_* \;. \end{aligned} \tag{2.71}$$

It then follows that,

$$\begin{aligned}
L\,g_m(v) &= -g_m(v)\ , \quad \text{for all odd } m. \\
L\,g_0(v) &= \quad 0 \\
L\,g_2(v) &= \quad 0 \\
L\,g_4(v) &= -\frac{1}{4}\big(v^4 - 6v^2 + 3\big) \\
L\,g_6(v) &= -\frac{3}{8}\big(v^6 - 5v^4 - 15v^2 + 15\big)\ , \text{ etc... }.
\end{aligned} \tag{2.72}$$

Suppose now that, the $h_k(v)$ is a polynomial of degree at most k, for $k > k_0$. From Eq. 2.70 it follows that h_{k_0+1} is a polynomial of degree at most $k_0 + 1$. This holds because S_{k_0} contains integrals of $h_{j-1}(v)\,h_{k_0+2-j}(v)$ $(j \geq 2)$, which is a polynomial of degree at most $k_0 + 1$. The same is easily verified for the remaining terms in the left hand side of Eq. 2.70. The result then follows from Eq. 2.72. And by induction it holds for all k.

For $k = 1, 2, \ldots$, at each ε^k level of Eq. 2.70, we use the conditions on the e_k, and the form of S_{k-1} as given in Eq. 2.69, and determine the first few terms of the unknown functions h_k to be

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

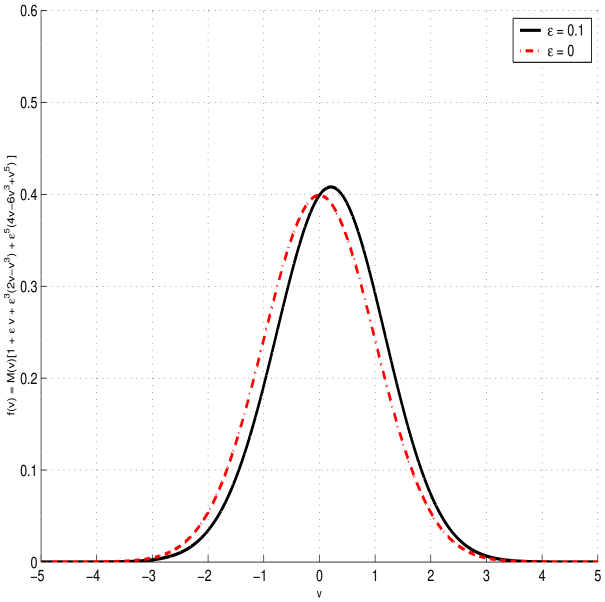
Setting these results back in $f_k = M h_k$, for $k = 1, 2, \ldots$, and recalling that $f_0 = M$, we justify the result that, for a small $\varepsilon > 0$

$$M(v)\ \Big(1 + \varepsilon v + \varepsilon^3\big(- v^3 + 2v\big) + \varepsilon^5\big(v^5 - 6v^3 + 4v\big) + \cdots\ \Big)\ , \tag{2.73}$$

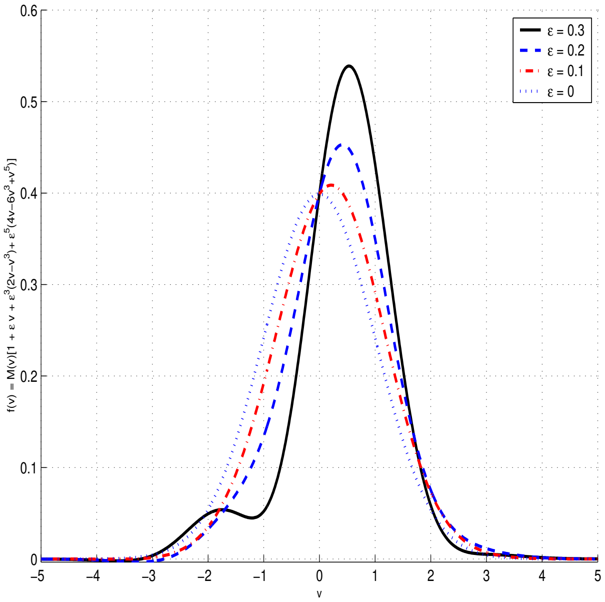
solves Eq. 2.33 asymptotically.

Part of this solution is plotted in Figure 2.2 for some values of ε. Also depicted in Figure 2.2 is the behaviour, as $\varepsilon \to 0$, of these non-equilibrium stationary state solutions tending to the Maxwellian, thereby recovering the usual solution to the underlying Boltzmann equation.

We recall that, the series expansion in Eq. 2.59 holds only for $\varepsilon < 0.5$. The various terms in that expansion were used in the development of the solution given in Eq. 2.73. With $\varepsilon \geq 0.5$, there is little hope that the asymptotic series in Eq. 2.73 will give good results. As depicted in Figure 2.2b, the truncated series may assume negative values, which clearly is unphysical.



a.



b.

Figure 2.2: Stationary state solutions and their behaviour for small ε.

Chapter 3

Simulation Results

3.1 Monte Carlo Methods for the Boltzmann Equation

The enormous mathematical difficulties involved in achieving exact analytical solutions on the one hand, and the inevitable need for practical calculations in rarefied gas dynamics on the other, have always been driving forces to the development of efficient computational techniques to the Boltzmann equation. Simulation procedures, both deterministic as well as stochastic type, of various levels of complexity have evolved along with the advent of powerful computers.

Monte Carlo (MC) methods, flourished in the 1960s and used in statistical physics where most quantities of interest are hard to compute exactly, have been instrumental in simulating real physical processes using sequences of random numbers. The basis for MC simulations is to construct a stochastic model in which the expected value of a certain random variable is equivalent to the value of some physical quantity to be determined. The expected value is then estimated by the average of many independent samples representing the random variable.

Applying MC methods to gas dynamics, Bird [4, 5] moved these techniques forward as he introduced, in the late 60s, the Direct Simulation Monte Carlo (DSMC) method. With this method he successfully simulated the structure of a normal shock wave and made calculations of shock profile which allowed meaningful comparisons with experimental results which were available at that time. Since then DSMC has been widely employed for the modelling of gas flows, where calculations are performed at a molecular level, through the computation of the motion and collisions of representative molecules.

The governing idea in DSMC is to construct a stochastic process for a many-particle system in such a way that the many-particle distribution at time $t > 0$ is close to the solution $f(t, \cdot, \cdot)$ of the Boltzmann equation. In so doing, the formalism of the integro-differential equation is bypassed, allowing instead a direct simulation of the physical situation that the equation describes.

In 1980, Nanbu [24] proposed a simulation procedure which was derived directly from the Boltzmann equation. Babovsky [1] made a slight modification or reinterpretation of this method. In 1989, Babovsky and Illner [2] rigorously proved that Nanbu's simulation method converges to solutions of the Boltzmann equation, when the number of test molecules go to infinity, if the exact solution is sufficiently smooth. In 1992, Wagner [30] proved that Bird's simulation method does indeed converge to solutions of the Boltzmann equation in a suitable limit. In Wagner's proof, which uses compactness arguments, use is made of the reinterpretation of the simulation scheme as a measure-valued stochastic process. Further details on the DSMC method, the underlying mathematical principles and its applications can be found in [6, 12].

Here we are not mainly focused on solving the Boltzmann equation, but rather the modified master equation. We also study how its solutions depend on the dimension of the equation, i.e. the number of 'particles'.

3.2 The Algorithm

Here we briefly describe the algorithm we used in the simulations. Fixed in this part of the description are the initial distribution, the collision frequency, the terminal time, and the number $N \geq 2$ of particles in the system.

i. Determine the number of expected collisions, and the next waiting time.

ii. Let all the particles evolve according to Eq. 2.9, i.e. effect of the thermostat.

iii. If it is time for a collision to occur,

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

   b. Choose a collision parameter θ, randomly from $[0, 2\pi)$.

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

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

iv. This is to be repeated, until the the terminal time is reached, using a new holding time, a new pair i and j, and a new scattering parameter θ; independently of everything that happened before.

3.3 Simulation Results

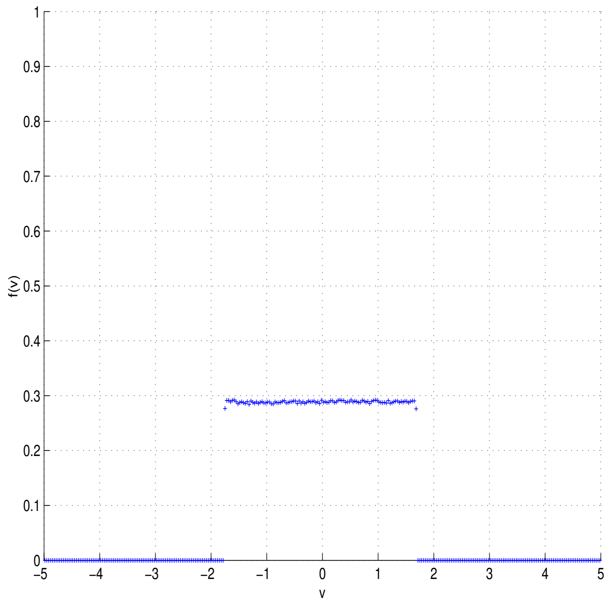
In this section we present results of our simulations. In line with the procedure described in the previous section, Monte Carlo simulations were performed. Throughout the simulations the collision frequency is fixed at $\frac{\sqrt{\pi}}{2}$, and the number of particles N in the simulation is taken to be $3, 10, 50, 100$ and 500. The magnitude of the force field E is made to vary from 0 to higher values.

We first consider the case $N = 3$, with no force field ($E = 0$). Figure 3.1a shows the resulting single-particle marginal to this setting. Using the result that $|S^2(\sqrt{3})| = 12\pi$ in Eq. 1.19, and normalising the resulting distribution then we get the constant single-particle marginal $f_1^3(v_1) = \frac{1}{2\sqrt{3}}$. This is in full agreement with the aforementioned simulation result. Figure 3.1b shows the uniform distribution of phase points over the surface $S^2(\sqrt{3})$.

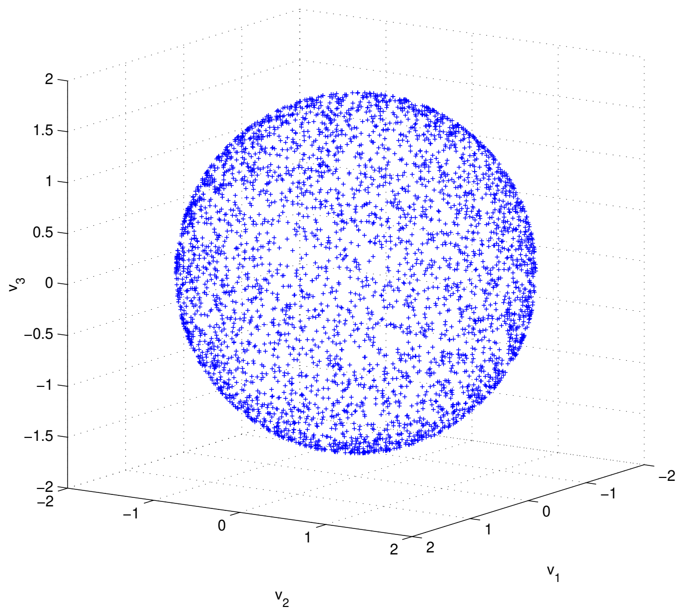
Figure 3.2 a and b show the single-particle marginals obtained as we apply force fields of magnitude $E = 0.5$ and $E = 1.0$, respectively, in to the dynamics. Setting the force field to relatively higher magnitudes, in Figure 3.3 a and b we present results showing the single-particle marginals, and the distribution of phase points over the surface $S^2(\sqrt{3})$ for $E = 1.5$. For $E = 2.0$ results are presented in Figure 3.4 a and b. Note that, when E is large, the field dominates over the collisions. The collisionless equlibria $v_i = 1$ (see Eq. 2.10) gives the curves of concentration in the figures.

To illustrate how good our simulation results resemble the limiting single-particle distribution function f, as $N \to \infty$, we set relatively bigger N's in the simulation. With $N = 50$ and force fields of magnitude 0.1, 0.5, and $\frac{1}{\sqrt{2}}$ we get the single-particle marginals depicted in Figure 3.5a. Figure 3.5b shows the result for force fields of magnitude 1.0, 1.5, and 2. The case $N = 500$ with $E = 0.10$, $E = 0.5$, and $E = \frac{1}{\sqrt{2}}$ is displayed in Figure 3.6a. Single-particle marginals corresponding to force fields of magnitude 1.0, 1.5, and 2 for $N = 500$ are presented in Figure 3.6b. To help us compare the effect of the force field, the case $E = 0$ was also considered in the simulation, resulting in the usual Maxwellian distribution (dotted lines) as indicated in all cases.

The steady current ζ was computed from the respective single-particle marginals corresponding to the different values of N with the indicated values of the force field E. We compare this computed current with the result from the exact analytical expression of ζ given in Eq. 2.37. These comparisons are presented in Figure 3.7, where a shows that for fields of magnitude between 0.1 and 1.0, while b is for those fields of strength between 1.0 and 3.0.

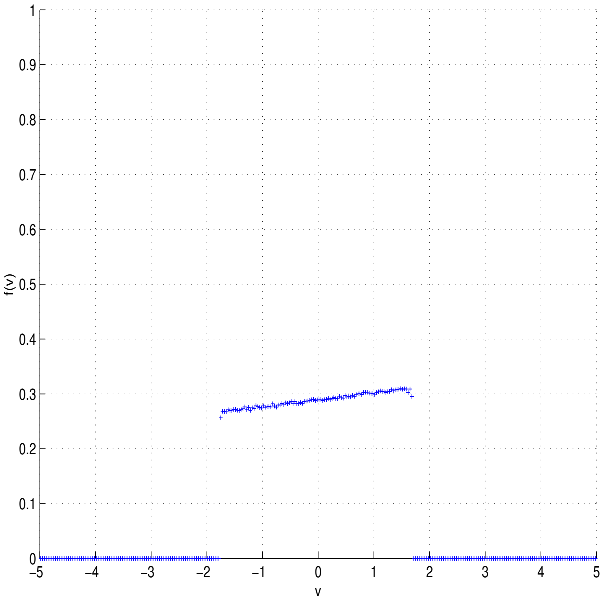


a.

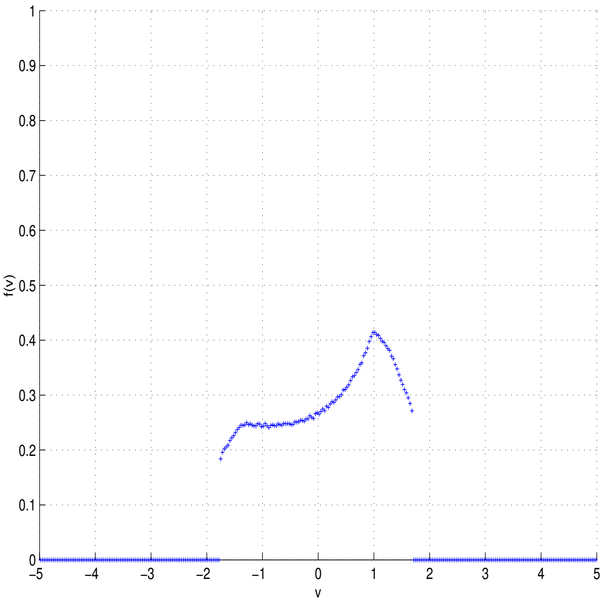


b.

Figure 3.1: Single-particle marginal(a) and phase space distribution(b) ($N = 3$, $E = 0$).

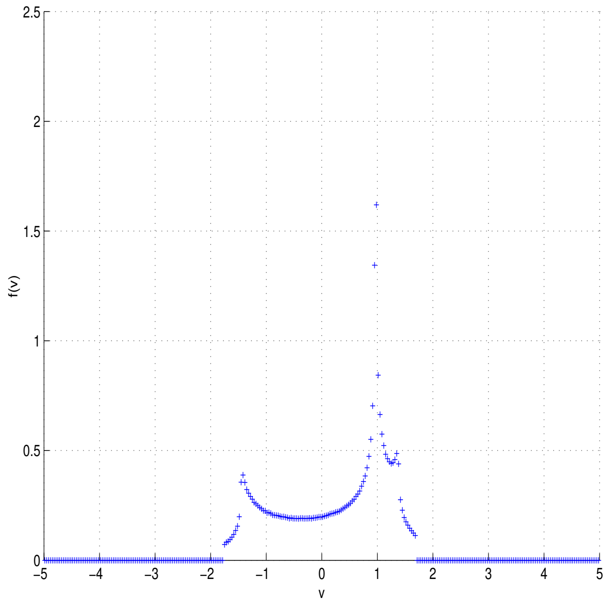


a.

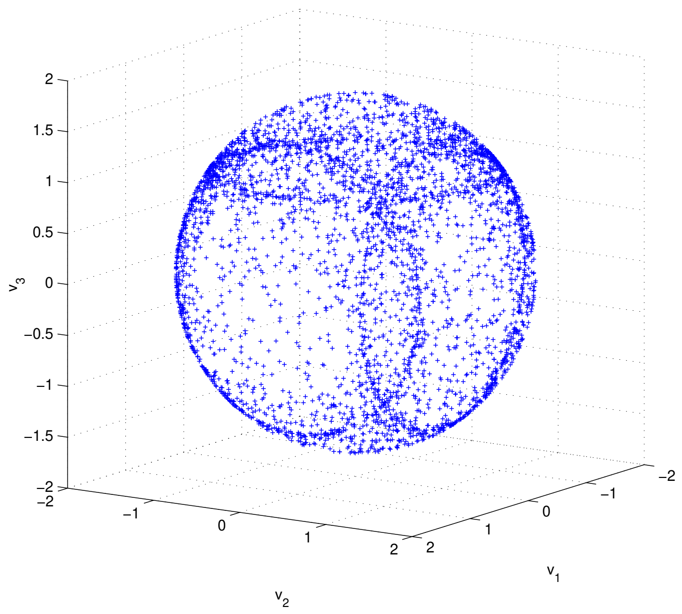


b.

Figure 3.2: Single-particle marginals ($N = 3$) a. $E = 0.1$, b. $E = 0.5$.

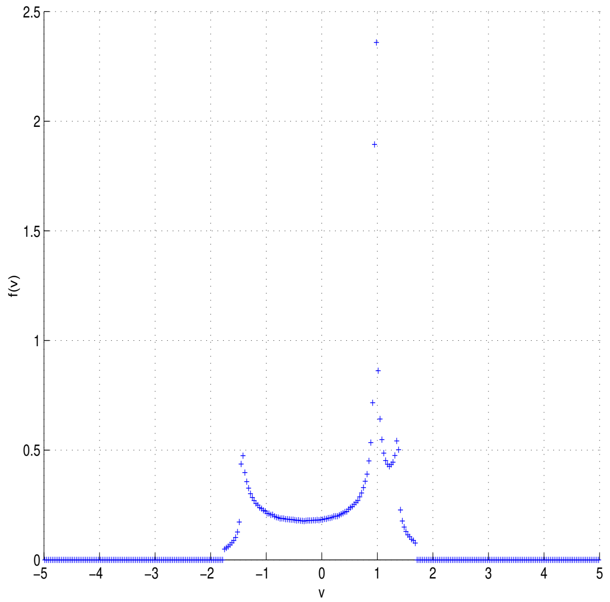


a.

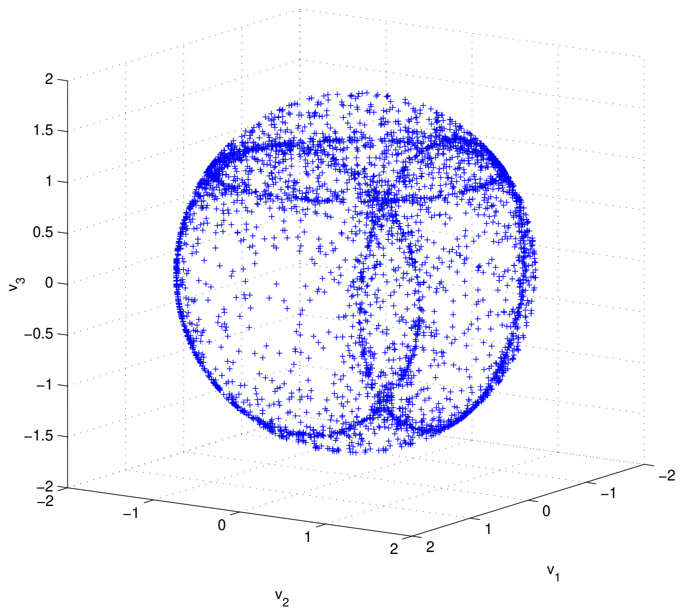


b.

Figure 3.3: Single-particle marginal and phase space distribution ($N = 3$, $E = 1.5$).

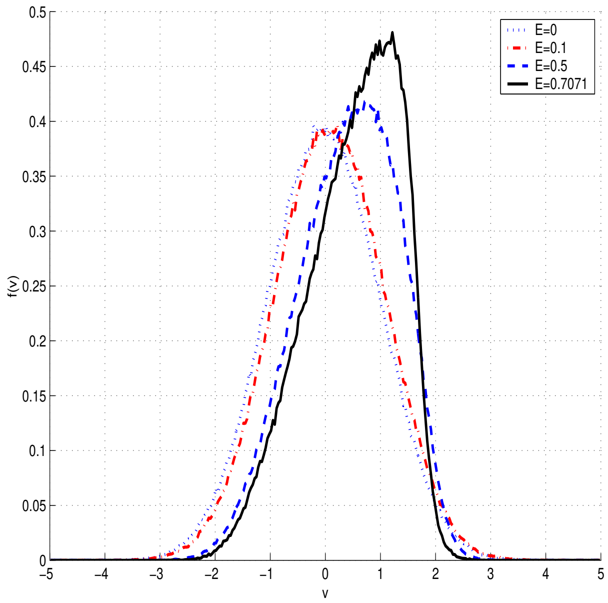


a.

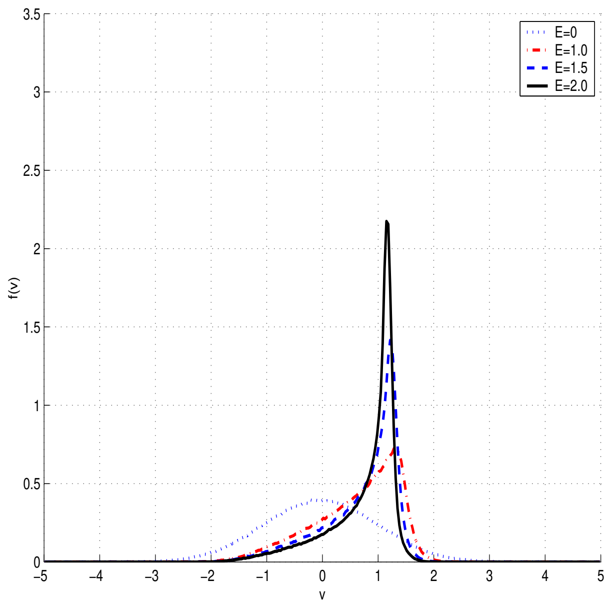


b.

Figure 3.4: Single-particle marginal and phase space distribution ($N = 3$, $E = 2.0$).

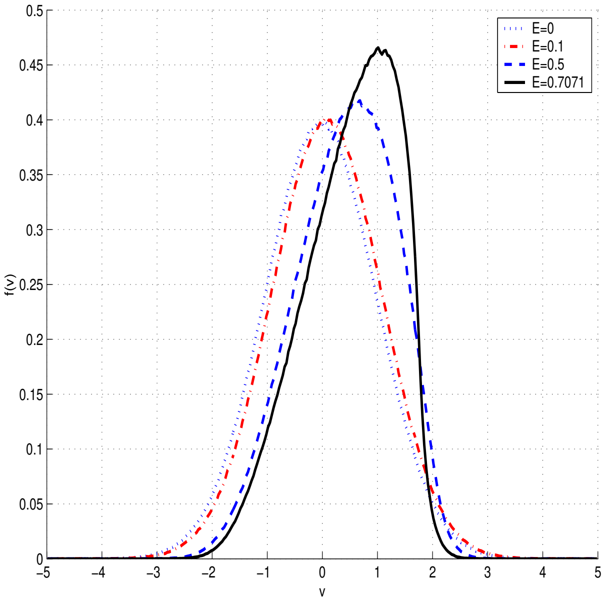


a.

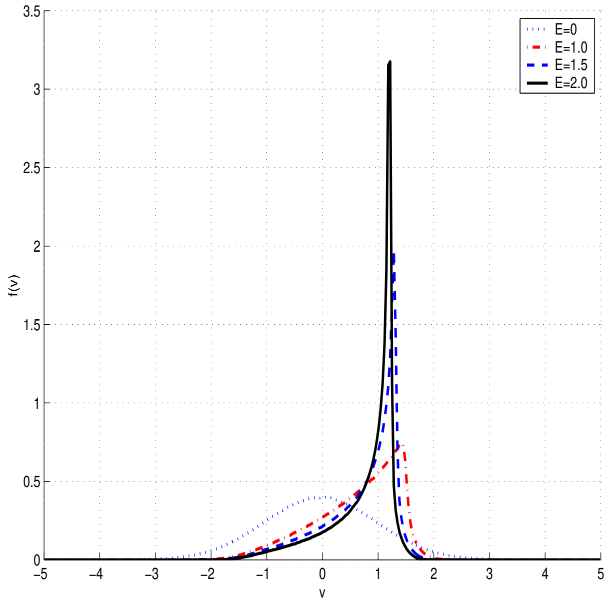


b.

Figure 3.5: Single-particle marginals (N=50).

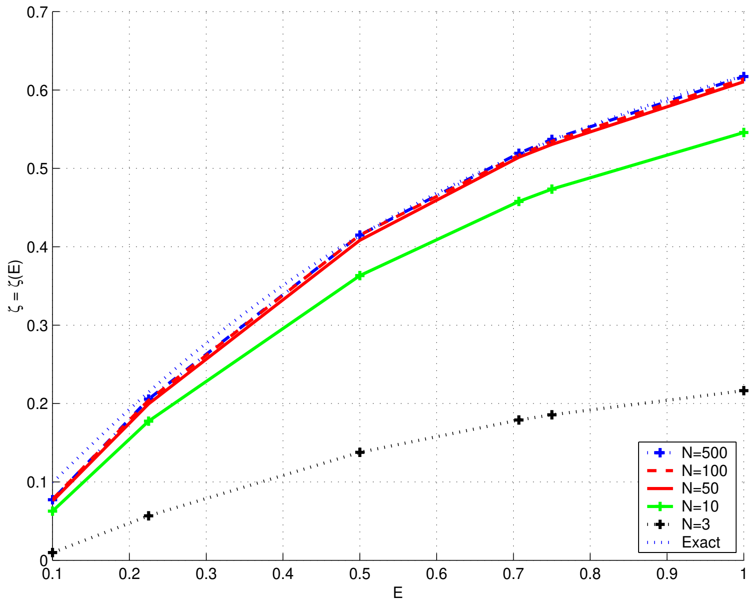


a.

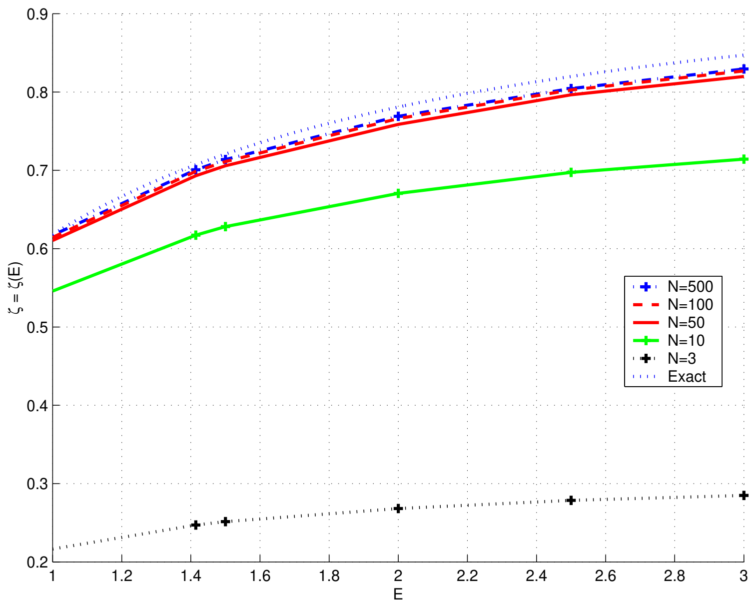


b.

Figure 3.6: Single-particle marginals (N=500).



a.



b.

Figure 3.7: Steady current as a function of E (N = 500, 100, 50, 10, 3).

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