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Carlo Cercignani

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Theory and Application to Micro-Electro-Mechanical Systems

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Preface

This volume is intended to cover the present status of the mathematical tools used to deal with problems related to slow rarefied flows. The meaning and usefulness of the subject, and the extent to which it is covered in the book, are discussed in some detail in the introduction. In short, I tried to present the basic concepts and the techniques used in probing mathematical questions and problems which arise when studying slow rarefied flows in environmental sciences and micromachines. For the book to be up-to-date without being excessively large, it was necessary to omit some topics, which are treated elsewhere, as indicated in the introduction and, whenever the need arises, in the various chapters of this volume. Their omission does not alter the aim of the book, to provide an understanding of the essential mathematical tools required to deal with slow rarefied flows and give the background for a study of the original literature.

Although I have tried to give a rather complete bibliographical coverage, the choice of the topics and of the references certainly reflects a personal bias and I apologize in advance for any omission.

I wish to thank Lorenzo Valdettaro, Antonella Abbà, Silva Lorenzani and Paolo Barbante for their help with pictures and especially Professor Ching Shen for his permission to reproduce his pictures on microchannel flows.

Milano, December 2005 Carlo Cercignani

Introduction

Rarefied gas dynamics can be defined as the study of gas flows in which the average value of the distance between two subsequent collisions of a molecule (the so-called mean free path) is not negligible in comparison with a length typical of the structure of the flow being considered, e.g., the thickness of a microchannel or the radius of curvature of the nose of a space shuttle. Thus it intrinsically requires the use of statistical ideas typical of the kinetic theory of gases as embodied in the integro-differential equation proposed by Boltzmann in 1872 and bearing his name.

Rarefied gas dynamics has existed, in principle, since the 19th century, but came in the foreground with space exploration. One can even give a birthdate, July 1958, when the first international symposium on rarefied gas dynamics was held in Nice (France). Since then, these symposia have been held regularly every second year. When glancing through the corresponding proceedings, one should not be surprised to find a shift of topics. The first few volumes contain a considerable amount of experimental papers and the theoretical papers contain very general surveys on the Boltzmann equation that rules the evolution of rarefied flows, but very few papers dealing with explicit solutions of some elementary problems. The first numerical solutions of some interest appear in 1962, but still in the late 1960s were few in number and not so accurate. Then one witnesses the reduction of experimental work and the increasing importance of numerical simulation. In the most recent volumes, experiments occupy just a few pages of the proceedings. This is compensated for by the fact that numerical simulations have spread through all the subfields, indicating the maturity reached by the theoretical understanding of the subject. Increasingly complicated phenomena, such as reacting flows or evaporation and condensation, are the object of widespread interest.

The mathematical theory of the Boltzmann equation goes back to such illustrious mathematicians as Hilbert and Carleman and is mentioned in the motivation of the Fields medal awarded to P.L. Lions in 1994. Some details of this theory will be presented in this book. The present introduction is mainly devoted to explain why this equation is so important for applications. We also remark that this book, although describing a well-defined topic, can serve two sets of readers: those more interested in the basic mathematical theory and those more interested in applications. The former might restrict themselves to Chapters 1–4, the latter to Chapter 1, the first section of Chapter 4 and Chapters 5–7.

In addition to space research, rarefied gas dynamics is also required in the area of environmental problems. Understanding and controlling the formation, motion, reactions and evolution of particles of varying composition and shapes, ranging from a diameter of the order of .001 μm to 50 μm, as well as their space-time distribution under gradients of concentration, pressure, temperature and the action of radiation, has grown in importance, because of the increasing awareness of the local and global problems related to the emission of particles from electric power plants, chemical plants, vehicles as well as of the role played by small particles in the formation of fog and clouds, in the release of radioactivity from nuclear reactor accidents, and in the problems arising from the exhaust streams of aerosol reactors, such as those used to produce optical fibers, catalysts, ceramics, silicon chips and carbon whiskers.

One cubic centimeter of atmospheric air at ground level contains approximately 2.5×10^{19} molecules. About a thousand of them may be charged (ions). A typical molecular diameter is 3×10^{-10} m (3×10^{-4} μm) and the average distance between the molecules is about ten times as much. The mean free path is of the order of 10^{-8} m, or 10^{-2} μm. In addition to molecules and ions, one cubic centimeter of air also contains a significant number of particles varying in size, as indicated above. In relatively clean air, the number of these particles can be 10^5 or more, including pollen, bacteria, dust, and industrial emissions. They can be both beneficial and detrimental, and arise from a number of natural sources as well as from the activities of all living organisms, especially humans. The particles can have complex chemical compositions and shapes, and may even be toxic or radioactive. A suspension of particles in a gas is known as an aerosol. Atmospheric aerosols are of global interest and have important impact on our lives. Aerosols are also of great interest in numerous scientific and engineering applications.

A third area of application of rarefied gas dynamics has emerged in the last few years and will be discussed in detail in the last chapter of the present book. Small size machines, called micromachines, are being designed and built. Their typical sizes range from a few microns to a few millimeters. Rarefied flow phenomena that are more or less laboratory curiosities in machines of more usual size can form the basis of important systems in the micromechanical domain. In fact, rarefied gas flows occur in many micro-electro-mechanical systems (MEMS), such as actuators, microturbines, gas chromatographs, and micro air vehicles (MAVs). A correct prediction of these flows is important to design and develop MEMS. Nanoscale design occurs for computer components as well and is no longer limited to chip technology but extends to mechanical devices as well. In a modern disk drive, the read/write head floats at distances of the order of 50 nm above the surface of the spinning platter. The prediction of the vertical force on the head (as obtained from the pressure distribution in the gas) is a crucial design calculation since the head will not accurately read or write if it flies too high. If the head flies too low, it can catastrophically collide against the platter. Micro-channels may have further computer applications because they are supposed to dissipate the heat generated in microchips more effectively than fans, and may be used as a more practical cooling system in integrated circuit chips.

Since, as these examples indicate, micro-devices are gaining popularity both in commercial applications and in scientific research, there exists a rapidly growing interest in improving the conventional design techniques related with these devices. Micro-devices are often operated in gaseous environments (typically air), and thus their performances are affected by the gas around them. The numerical simulation of all these flows cannot be performed with the Navier–Stokes equations (or the related Reynolds equation for a slider air bearing) because the smallest characteristic length of MEMS or of the thin air film occurring in a computer drive is comparable with (or smaller than) the mean free path of the gas molecules. For this reason the continuum equations are no longer valid and the Boltzmann equation must be invoked to understand and compute the rarefied flows related to these devices.

Numerical methods based on this equation are generally numerically expensive especially when the flow to be considered progresses from free molecular, through transitional, to continuum regions. Since these flows, contrary to the flow past space vehicles, are usually at low Mach number, the use of the linearized Boltzmann equation is permissible and this revives old methods developed in the sixties and seventies of the 20th century to deal with this equation.

Among the rarefied flows of interest, one should not forget the design and simulation of the aerosol reactors, used to produce optical fibers, catalysts, ceramics, silicon chips and carbon whiskers, which have been mentioned above as sources of air pollution. A further area of interest occurs in the vacuum industry. Although this area has existed for a long time, the expense of the early computations with kinetic theory precluded applications of numerical methods. The latter could develop only in the context of the aerospace industry, because the big budgets required till recently were available only there.

The present volume is an attempt to cover the mathematical results and techniques to deal with rarefied flows when the speeds are small with respect to the sound speed. The mathematical theory is much more advanced in this case and provides a rigorous justification for the use of the linearized Boltzmann equation, which avoids costly simulations based on Monte Carlo methods.

After introducing the Boltzmann equation in Chapter 1, we shall survey the rigorous theorems on validity and existence in Chapter 2. Chapter 3 is devoted to the basic existence theory for flows close to equilibria in an infinite expanse of gas or in a periodic box. Chapter 4 deals with more realistic boundary conditions and Chapter 5 deals with the techniques used to solve problems in the simple but extremely important case of a slab geometry. Chapter 6 discusses problems in three dimensions and Chapter 7 is devoted to the recent contributions to rarefied lubrication theory with particular attention to applications to MEMS.

Chapter 1

The Boltzmann Equation

1.1 Historical Introduction

In 1738 Daniel Bernoulli advanced the idea that gases are formed of elastic molecules rushing hither and thither at large speeds, colliding and rebounding according to the laws of elementary mechanics. Of course, this was not a completely new idea, because several Greek philosophers asserted that the molecules of all bodies are in motion even when the body itself appears to be at rest. The new idea was that the mechanical effect of the impact of these moving molecules when they strike against a solid is what is commonly called the pressure of the gas. In fact if we were guided solely by the atomic hypothesis, we might suppose that the pressure would be produced by the repulsions of the molecules. Although Bernoulli's scheme was able to account for the elementary properties of gases (compressibility, tendency to expand, rise of temperature in a compression and fall in an expansion, trend toward uniformity), no definitive opinion could be passed on it until it was investigated quantitatively. The actual development of the kinetic theory of gases was, accordingly, accomplished much later, in the nineteenth century.

Frequently the molecules of a gas can be assumed to be perfectly elastic spheres that move according to the laws of classical mechanics. Thus, e.g., if no external force, such as gravity, is assumed to act on the molecules, each of them will move in a straight line unless it happens to strike another sphere or a solid wall. Systems of this kind are usually called billiards, for obvious reasons.

Although the rules generating the dynamics of these systems are easy to prescribe, the phenomena associated with this dynamics are not so simple. They are actually rather difficult to understand, especially if one is interested in the asymptotic behavior of the system for long times (ergodic properties) or in the case when the number of spheres is very large (kinetic and hydrodynamical limits). Both aspects of the dynamics of hard spheres are relevant when dealing with a gas, but we shall now concentrate upon the problem of outlining the behavior of this system when the number of the particles is very large. This is due to the fact that there are about $2.7 \cdot 10^{19}$ molecules in a cubic centimeter of a gas at atmospheric pressure and a temperature of $0°$C.

Given the enormous number of particles to be considered, it would of course be a perfectly hopeless task to attempt to describe the state of the gas by specifying the so-called microscopic state, i.e., the position and velocity of every individual particle, and we must have recourse to statistics. This is possible because in practice all that our observation can detect are changes in the macroscopic state of the gas, described by quantities such as density, velocity, temperature, stresses, heat flow, which are related to the suitable averages of quantities depending on the microscopic state.

In 1866 James Clerk Maxwell (1831–1879) developed an accurate method[24], based on the so-called transfer equations, and discovered the particularly simple properties of a model, according to which the molecules interact at a distance with a force inversely proportional to the fifth power of the distance (nowadays commonly called Maxwellian molecules). In the same paper he gave a justification of his earlier formula for the velocity distribution function for a gas in equilibrium.

With his transfer equations, Maxwell had come very close to an evolution equation for the distribution, but this step[4] must be credited to Ludwig Boltzmann (1844–1906). The equation under consideration is usually called the Boltzmann equation and sometimes the Maxwell–Boltzmann equation (to recognize the important role played by Maxwell in its discovery).

In the same paper, where he gave a heuristic derivation of his equation, Boltzmann deduced an important consequence from it, which later came to be known as the H-theorem. This theorem attempts to explain the irreversibility of natural processes in a gas, by showing how molecular collisions tend to increase entropy. The theory was attacked by several physicists and mathematicians in the 1890s, because it appeared to produce paradoxical results. However, within a few years of Boltzmann's suicide in 1906, the existence of atoms had been firmly established by experiments such as those on Brownian motion.

The paradoxes indicate, however, that some reinterpretation is necessary. Boltzmann himself had proposed that the H-theorem be interpreted statistically; later, Paulus Ehrenfest (1880–1933), together with his wife Tatiana, gave a brilliant analysis of the matter, which elucidated Boltzmann's ideas and made it highly plausible, at least from a heuristic standpoint. A rigorous analysis, however, had still to come.

In the meantime, the Boltzmann equation had become a practical tool for investigating the properties of dilute gases. In 1912 the great mathematician David Hilbert (1862–1943) indicated[19] how to obtain approximate solutions of the Boltzmann equation by a series expansion in a parameter, inversely proportional to the gas density. The paper is also reproduced as Chapter XXII of his treatise entitled *Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen.* The reasons for this are clearly stated in the preface of the book ("Neu hinzugefügt habe ich zum Schluss ein Kapitel über kinetische Gastheorie. [...] erblicke ich in der Gastheorie die glänzendste Anwendung der die Auflösung der Integralgleichungen betreffenden Theoreme").

In about the same year (1916–1917) Sidney Chapman[12] (1888–1970) in England and David Enskog[14] (1884–1947) in Sweden independently obtained approximate solutions of the Boltzmann equation, valid for a sufficiently dense gas. The results were identical as far as practical applications were concerned, but the methods differed widely in spirit and detail. Enskog presented a systematic technique generalizing Hilbert's idea, while Chapman simply extended a method previously indicated by Maxwell to obtain transport coefficients. Enskog's method was adopted by S. Chapman and T. G. Cowling in their book *The Mathematical Theory of Non-uniform Gases* and thus became to be known as the Chapman–Enskog method.

Then for many years no essential progress in solving the equation came. Rather the ideas of kinetic theory found their way in other fields, such as radiative transfer, the theory of ionized gases and, subsequently, in the the theory of neutron transport. Almost unnoticed, however, the rigorous theory of the Boltzmann equation had started in 1933 with a paper[5] by Tage Gillis Torsten Carleman (1892–1949), who proved a theorem of global existence and uniqueness for a gas of hard spheres in the so-called space homogeneous case. The theorem was proved under the restrictive assumption that the initial data depend upon the molecular velocity only through its magnitude. This restriction is removed in a posthumous book by the same author[6].

In 1949 Harold Grad (1923–1986) wrote a paper[17], which became widely known because it contained a systematic method of solving the Boltzmann equation by expanding the solution into a series of orthogonal polynomials. In the same paper, however, Grad made a more basic contribution to the theory of the Boltzmann equation for molecules of diameter σ. In fact, he formulated a conjecture on the validity of the Boltzmann equation. In his words: "From the preceding discussion it is possible to see along what lines a rigorous derivation of the Boltzmann equation should proceed. First, from equilibrium considerations we must let the number density of molecules, N, increase without bound. At the same time we would like the macroscopic properties of the gas to be unchanged. To do this we allow m to approach zero in such a way that $mN = \rho$ is fixed. The Boltzmann equation for elastic spheres, (2.37) has a factor σ^2/m in the collision term. If σ is made to approach to zero at such a rate that σ^2/m is fixed, then the Boltzmann equation remains unaltered. [...] In the limiting process described here, it seems likely that solutions of Liouville's equation attain many of the significant properties of the Boltzmann equation."

In the 1950s there were some significant results concerning the Boltzmann equation. A few exact solutions were obtained by C. Truesdell[28] in the U.S.A. and by V. S. Galkin[15,16] in the Soviet Union, while the existence theory was extended by D. Morgenstern[25], who proved a global existence theorem for a gas of Maxwellian molecules in the space homogeneous case. His work was extended by L. Arkeryd[1,2] in 1972.

In the 1960s, under the impact of the problems related to space research, the main interest was in the direction of finding approximate solutions of the Boltzmann equation and developing mathematical results for the perturbation of equilibrium[7,8]. Important methods developed by H. Grad[18] were brought to completion much later by S. Ukai, Y. Shizuta, K. Asano, T. Nishida and K. Imai[26,27,29].

The problem of proving the validity of the Boltzmann equation was still completely open. In 1972, C. Cercignani[9] proved that taking the limit indicated by Grad in the passage quoted above (now currently called the Boltzmann–Grad limit) produced, from a formal point of view, a perfectly consistent theory, i.e., the so-called Boltzmann hierarchy. This result clearly indicated that the difficulties of the rigorous derivation of the Boltzmann equation were not of a formal nature but were at least of the same order of difficulty as those of proving theorems of existence and uniqueness in the space inhomogeneous case. Subsequently, O. Lanford proved[23] that the formal derivation becomes rigorous if one limits himself to a sufficiently short time interval. The problem of a rigorous, globally valid justification of the Boltzmann equation is still open, except for the case of an expanding rare cloud of gas in a vacuum, for which the difficulties were overcome by R. Illner and M. Pulvirenti[20,21], after Illner and Shinbrot had provided the corresponding existence and uniqueness theorem for the Boltzmann equation[22].

More recently, R. Di Perna and P. L. Lions[13] have proved a global existence theorem for quite general data, but several important problems, such as proving that energy is conserved or controlling the growth of density are still open.

1.2 The Boltzmann Equation

The phenomena associated with the dynamics of molecules are not so simple, especially because the number of molecules usually considered is extremely large: there are about $2.7 \cdot 10^{19}$ in a cubic centimeter of a gas at atmospheric pressure and a temperature of $0°$C.

Given the vast number of particles to be considered, it would of course be a hopeless task to attempt to describe the state of the gas by specifying the so-called microscopic state, i.e., the position and velocity of every individual sphere; we must have recourse to statistics. A description of this kind is made possible because in practice all that our typical observations can detect are changes in the macroscopic state of the gas, described by quantities such as density, bulk velocity, temperature stresses, heat flow, which are related to some suitable averages of quantities depending on the microscopic state.

The exact dynamics of N particles is a useful conceptual tool, but cannot in any way be used in practical calculations because it requires a huge number of real variables (of the order of 10^{20}). This was realized by Maxwell and Boltzmann when they started to work with the one-particle probability density, or distribution function $P^{(1)}(\mathbf{x}, \boldsymbol{\xi}, t)$. The latter is a function of seven variables, i.e., the components of the two vectors $\mathbf{x}$ and $\boldsymbol{\xi}$ and time t. In particular, Boltzmann wrote an evolution equation for $P^{(1)}$ by means of a heuristic argument, which we shall try to present in such a way as to show where extra assumptions are introduced.

Let us first consider the meaning of $P^{(1)}(\mathbf{x}, \boldsymbol{\xi}, t)$; it gives the probability density of finding one fixed particle (say, the one labelled by 1) at a certain point $(\mathbf{x}, \boldsymbol{\xi})$ of the six-dimensional reduced phase space associated with the position and velocity of that molecule. In order to simplify the treatment, we shall for the moment assume that the molecules are hard spheres, whose center has position $\mathbf{x}$. When the molecules collide, momentum and kinetic energy must be conserved; thus the velocities after the impact, $\boldsymbol{\xi}_1'$ and $\boldsymbol{\xi}_2'$, are related to those before the impact, $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$, by

$$\begin{aligned} \boldsymbol{\xi}_1' &= \boldsymbol{\xi}_1 - \mathbf{n}[\mathbf{n} \cdot (\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2)], \\ \boldsymbol{\xi}_2' &= \boldsymbol{\xi}_2 + \mathbf{n}[\mathbf{n} \cdot (\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2)] \end{aligned} \tag{1.2.1}$$

where $\mathbf{n}$ is the unit vector along $\boldsymbol{\xi}_1 - \boldsymbol{\xi}_1'$. Note that the relative velocity

$$\mathbf{V} = \boldsymbol{\xi}_1 - \boldsymbol{\xi}_2 \tag{1.2.2}$$

satisfies

$$\mathbf{V}' = \mathbf{V} - 2\mathbf{n}(\mathbf{n} \cdot \mathbf{V}) \tag{1.2.3}$$

i.e., undergoes a specular reflection at the impact. This means that if we split $\mathbf{V}$ at the point of impact into a normal component $\mathbf{V}_n$, directed along $\mathbf{n}$ and a tangential component $\mathbf{V}_t$ (in the plane normal to $\mathbf{n}$), then $\mathbf{V}_n$ changes sign and $\mathbf{V}_t$ remains unchanged in a collision. We can also say that $\mathbf{n}$ bisects the directions of $\mathbf{V}$ and $-\mathbf{V}' = -(\boldsymbol{\xi}_1' - \boldsymbol{\xi}_2')$ (see Fig. 1.1).

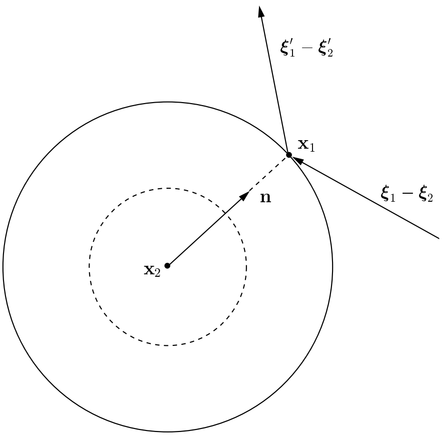

Figure 1.1: The directions of the relative velocities before and after the impact are bisected by the unit vector $\mathbf{n}$.

Let us remark that, in the absence of collisions, $P^{(1)}$ would remain unchanged along the trajectory of a particle and would satisfy

$$\frac{\partial P^{(1)}}{\partial t} + \boldsymbol{\xi}_1 \cdot \frac{\partial P^{(1)}}{\partial \mathbf{x}_1} + \mathbf{X}_1 \cdot \frac{\partial P^{(1)}}{\partial \boldsymbol{\xi}_1} = 0$$

where $\mathbf{X}_1$ is any external force per unit mass, such as gravity, acting on the molecule, which will be neglected in the rest of the book.

We must now evaluate the effects of collisions on the time evolution of $P^{(1)}$. Note that the probability of occurrence of a collision is related to the probability of finding another molecule with a center at exactly one diameter from the center of the first one, whose distribution function is $P^{(1)}$. Thus, generally speaking, in order to write the evolution equation for $P^{(1)}$ we shall need another function, $P^{(2)}$, which gives the probability density of finding, at time t, the first molecule at $\mathbf{x}_1$ with velocity $\boldsymbol{\xi}_1$ and the second at $\mathbf{x}_2$ with velocity $\boldsymbol{\xi}_2$; obviously $P^{(2)} = P^{(2)}(\mathbf{x}_1, \mathbf{x}_2, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)$. Hence $P^{(1)}$ satisfies an equation of the form

$$\frac{\partial P^{(1)}}{\partial t} + \boldsymbol{\xi}_1 \cdot \frac{\partial P^{(1)}}{\partial \mathbf{x}_1} = G - L. \tag{1.2.4}$$

Here $Ld\mathbf{x}_1 d\boldsymbol{\xi}_1 dt$ gives the expected number of particles with position between $\mathbf{x}_1$ and $\mathbf{x}_1 + d\mathbf{x}_1$ and velocity between $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_1 + d\boldsymbol{\xi}_1$ which disappear from these ranges of values because of a collision in the time interval between t and $t + dt$, and $Gd\mathbf{x}_1 d\boldsymbol{\xi}_1 dt$ gives the analogous number of particles entering the same range in the same time interval. The count of these numbers is easy, provided we use the trick of imagining particle 1 as a sphere at rest and endowed with twice the actual diameter σ and the other particles to be point masses with velocity $(\boldsymbol{\xi}_i - \boldsymbol{\xi}_1) = \mathbf{V}_i$. In fact, each collision will send particle 1 out of the above range and the number of the collisions of particle 1 will be the number of expected collisions of any other particle with that sphere. Since there are exactly $(N - 1)$ identical point masses and multiple collisions can be disregarded (because they form a set of measure zero in the set of collisions), $G = (N - 1)g$ and $L = (N - 1)l$, where the lower case letters indicate the contribution of a fixed particle, say particle 2. We shall then compute the effect of the collisions of particle 2 with particle 1. Let $\mathbf{x}_2$ be a point of the sphere such that the vector joining the center of the sphere with $\mathbf{x}_2$ is $\sigma\mathbf{n}$, where $\mathbf{n}$ is a unit vector. A cylinder with height $|\mathbf{V} \cdot \mathbf{n}|dt$ (where we write just $\mathbf{V}$ for $\mathbf{V}_2$) and base area $dS = \sigma^2 d\mathbf{n}$ (where $d\mathbf{n}$ is the area of a surface element of the unit sphere about $\mathbf{n}$) will contain the particles with velocity $\boldsymbol{\xi}_2$ hitting the base dS in the time interval $(t, t + dt)$ (see Fig. 1.2); its volume is $\sigma^2 d\mathbf{n}|\mathbf{V} \cdot \mathbf{n}|dt$. Thus the number of collisions of particle 2 with particle 1 in the ranges $(\mathbf{x}_1, \mathbf{x}_1 + d\mathbf{x}_1), (\boldsymbol{\xi}_1, \boldsymbol{\xi}_1 + d\boldsymbol{\xi}_1), (\mathbf{x}_2, \mathbf{x}_2 + d\mathbf{x}_2), (\boldsymbol{\xi}_2, \boldsymbol{\xi}_2 + d\boldsymbol{\xi}_2), (t, t + dt)$ occurring at points of dS is $P^{(2)}(\mathbf{x}_1, \mathbf{x}_2, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)d\mathbf{x}_1 d\boldsymbol{\xi}_1 d\boldsymbol{\xi}_2 x\sigma^2 d\mathbf{n}|\mathbf{V} \cdot \mathbf{n}|\mathrm{dt}$. If we want the number of collisions of particle 1 with 2, when the range of the former is fixed but the latter may have any velocity $\boldsymbol{\xi}_2$ and any position $\mathbf{x}_2$ on the sphere (i.e., any $\mathbf{n}$), we integrate over the sphere and all the possible velocities of particle 2 to obtain:

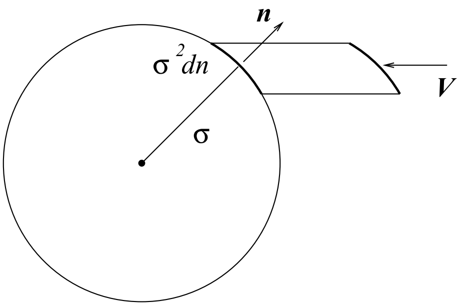

Figure 1.2: Calculation of the number of collisions between two molecules.

$$ld\mathbf{x}_1 d\boldsymbol{\xi}_1 dt = d\mathbf{x}_1 d\boldsymbol{\xi}_1 dt \int_{R^3}\int_{\mathcal{B}^-} P^{(2)}(\mathbf{x}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)|\mathbf{V}\cdot\mathbf{n}|\sigma^2 d\mathbf{n} d\boldsymbol{\xi}_2 \quad (1.2.5)$$

where $\mathcal{B}^-$ is the hemisphere corresponding to $\mathbf{V}\cdot\mathbf{n} < 0$ (the particles are moving one toward the other before the collision). Thus we have the following result:

$$L = (N-1)\sigma^2 \int_{R^3}\int_{\mathcal{B}^-} P^{(2)}(\mathbf{x}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n}. \quad (1.2.6)$$

The calculation of the gain term G is exactly the same as the one for L, except for the fact that we have to integrate over the hemisphere B^+, defined by $\mathbf{V}\cdot\mathbf{n} > 0$ (the particles are moving away one from the other after the collision). Thus we have:

$$G = (N-1)\sigma^2 \int_{R^3}\int_{\mathcal{B}^+} P^{(2)}(\mathbf{x}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n}. \quad (1.2.7)$$

We thus could write the right-hand side of Eq. (1.2.4) as a single expression:

$$G - L = (N-1)\sigma^2 \int_{R^3}\int_{\mathcal{B}} P^{(2)}(\mathbf{x}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, t)(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n} d\boldsymbol{\xi}_2 d\mathbf{n} \quad (1.2.8)$$

where now $\mathcal{B}$ is the entire unit sphere and we have abolished the bars of absolute value in the right-hand side.

Eq. (1.2.8), although absolutely correct, is not so useful. It turns out that it is much more convenient to keep the gain and loss terms separated. Only in this way, in fact, can we insert in Eq. (1.2.4) the information that the probability density $P^{(2)}$ is continuous at a collision; in other words, although the velocities of the particles undergo the discontinuous change described by Eqs. (1.2.1), we can write:

$$P^{(2)}(\mathbf{x}_1, \boldsymbol{\xi}_1, \mathbf{x}_2, \boldsymbol{\xi}_2, t) = P^{(2)}(\mathbf{x}_1, \boldsymbol{\xi}_1 - \mathbf{n}(\mathbf{n}\cdot\mathbf{V}), \mathbf{x}_2, \boldsymbol{\xi}_2 + \mathbf{n}(\mathbf{n}\cdot\mathbf{V}), t),$$
$$\text{if } |\mathbf{x}_1 - \mathbf{x}_2| = \sigma. \quad (1.2.9)$$

For brevity, we write (in agreement with Eq. (1.2.1):

$$\boldsymbol{\xi}_1' = \boldsymbol{\xi}_1 - \mathbf{n}(\mathbf{n}\cdot\mathbf{V}) \qquad \boldsymbol{\xi}_2' = \boldsymbol{\xi}_2 + \mathbf{n}(\mathbf{n}\cdot\mathbf{V}). \tag{1.2.10}$$

Inserting Eq. (1.2.8) in Eq. (1.2.5) we thus obtain:

$$G = (N-1)\sigma^2 \int_{R^3}\int_{\mathcal{B}^+} P^{(2)}(\mathbf{x}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_1', \boldsymbol{\xi}_2', t)|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n} \tag{1.2.11}$$

which is a frequently used form. Sometimes $\mathbf{n}$ is changed into $-\mathbf{n}$ in order to have the same integration range as in L; the only change (in addition to the change in the range) is in the second argument of $P^{(2)}$, which becomes $\mathbf{x}_1 - \sigma\mathbf{n}$.

At this point we are ready to understand Boltzmann's argument. N is a very large number and σ (expressed in common units, such as, e.g., centimeters) is very small; to fix the ideas, let us consider a box whose volume is 1 cm^3 at room temperature and atmospheric pressure.Then $N \cong 10^{20}$ and $\sigma \cong 10^{-8}$cm. Then $(N-1)\sigma^2 \cong N\sigma^2 \cong 10^4 cm^2 = 1m^2$ is a sizable quantity, while we can neglect the difference between $\mathbf{x}_1$ and $\mathbf{x}_1 + \sigma\mathbf{n}$. This means that the equation to be written can be rigorously valid only in the so-called *Boltzmann–Grad limit*, when $N \to \infty, \sigma \to 0$ with $N\sigma^2$ finite.

In addition, the collisions between two preselected particles are rather rare events. Thus two spheres that happen to collide can be thought to be two randomly chosen particles and it makes sense to assume that the probability density of finding the first molecule at $\mathbf{x}_1$ with velocity $\boldsymbol{\xi}_1$ and the second at $\mathbf{x}_2$ with velocity $\boldsymbol{\xi}_2$ is the product of the probability density of finding the first molecule at $\mathbf{x}_1$ with velocity $\boldsymbol{\xi}_1$ times the probability density of finding the second molecule at $\mathbf{x}_2$ with velocity $\boldsymbol{\xi}_2$. If we accept this we can write (assumption of *molecular chaos*):

$$P^{(2)}(\mathbf{x}_1, \boldsymbol{\xi}_1, \mathbf{x}_2, \boldsymbol{\xi}_2, t) = P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1, t)P^{(1)}(\mathbf{x}_2, \boldsymbol{\xi}_2, t) \tag{1.2.12}$$

for two particles that are about to collide, or:

$$P^{(2)}(\mathbf{x}_1, \boldsymbol{\xi}_1, \mathbf{x}_1 + \sigma\mathbf{n}, \boldsymbol{\xi}_2, t) = P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1, t)P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2, t)$$
$$\text{for} \quad (\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n} < 0. \tag{1.2.13}$$

Thus we can apply this *recipe* to the loss term (1.2.4) but not to the gain term in the form (1.2.5). It is possible, however, to apply Eq. (1.2.13) (with $\boldsymbol{\xi}_1', \boldsymbol{\xi}_2'$ in place of $\boldsymbol{\xi}_1, \boldsymbol{\xi}_2$) to the form (1.2.9) of the gain term, because the transformation (1.2.10) maps the hemisphere $\mathcal{B}^+$ onto the hemisphere $\mathcal{B}^-$.

If we accept all the simplifying assumptions made by Boltzmann, we obtain the following form for the gain and loss terms:

$$G = N\sigma^2 \int_{R^3}\int_{\mathcal{B}^-} P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1', t)P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2', t)|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n}, \tag{1.2.14}$$

$$L = N\sigma^2 \int_{R^3}\int_{\mathcal{B}^-} P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1, t)P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2, t)|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1)\cdot\mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n}. \tag{1.2.15}$$

By inserting these expressions in Eq. (1.2.6) we can write the *Boltzmann equation* in the form

$$\frac{\partial P^{(1)}}{\partial t} + \boldsymbol{\xi}_1 \cdot \frac{\partial P^{(1)}}{\partial \mathbf{x}_1} = N\sigma^2 \int_{R^3} \int_{\mathcal{B}^-} [P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1', t) P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2', t)$$
$$- P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1, t) P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2, t)] |(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1) \cdot \mathbf{n}| d\boldsymbol{\xi}_2 d\mathbf{n}. \tag{1.2.16}$$

We remark that the expressions for $\boldsymbol{\xi}_1'$ and $\boldsymbol{\xi}_2'$ given in Eq. (1.2.1) are by no means the only possible ones. In fact we might use a different unit vector $\boldsymbol{\omega}$, directed as $\mathbf{V}'$, instead of $\mathbf{n}$. Then Eq. (1.2.1) is replaced by:

$$\boldsymbol{\xi}_1' = \overline{\boldsymbol{\xi}} + \frac{1}{2}|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2|\boldsymbol{\omega},$$
$$\boldsymbol{\xi}_2' = \overline{\boldsymbol{\xi}} - \frac{1}{2}|\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2|\boldsymbol{\omega} \tag{1.2.17}$$

where $\overline{\boldsymbol{\xi}} = \frac{1}{2}(\boldsymbol{\xi}_1 + \boldsymbol{\xi}_2)$ is the velocity of the center of mass. The relative velocity $\mathbf{V}$ satisfies

$$\mathbf{V}' = \boldsymbol{\omega}|\mathbf{V}|. \tag{1.2.18}$$

The Boltzmann equation is an evolution equation for $P^{(1)}$, without any reference to $P^{(2)}$. This is its main advantage. However, it has been obtained at the price of several assumptions; the chaos assumption present in Eqs. (1.2.12) and (1.2.13) is particularly strong and requires to be discussed.

The molecular chaos assumption is clearly a property of randomness. Intuitively, one feels that collisions exert a randomizing influence, but it would be completely wrong to argue that the statistical independence described by Eq. (1.2.12) is a consequence of the dynamics. It is quite clear that we cannot expect every choice of the initial distribution of positions and velocities of the molecules to give a $P^{(1)}$ which agrees with the solution of the Boltzmann equation in the Boltzmann–Grad limit. In other words molecular chaos must be present initially and we can only ask whether it is preserved by the time evolution of the system of hard spheres.

It is evident that the chaos property (1.2.12), if initially present, is almost immediately destroyed, if we insist that it should be valid everywhere. In fact, if it were strictly valid everywhere, the gain and loss terms, in the Boltzmann–Grad limit, would be exactly equal. As a consequence, there would be no effect of the collisions on the time evolution of $P^{(1)}$. The essential point is that we need the chaos property only for molecules which are about to collide, i.e., in the precise form stated in Eq. (1.2.13). It is clear then that even if $P^{(1)}$ as predicted by the exact dynamics converges nicely to a solution of the Boltzmann equation, $P^{(2)}$ may converge to a product, as stated in Eq. (1.2.11), only in a way which is in a certain sense very singular. In fact, it is not enough to show that the convergence is almost everywhere, because we need to use the chaos property in a zero measure set. On the other hand we cannot try to show that convergence holds everywhere, because this would be false; in fact, we have just remarked that Eq. (1.2.11) is, generally speaking, simply not true for molecules which have just collided.

How can we approach the question of justifying the Boltzmann equation without invoking the molecular chaos assumption as an *a priori* hypothesis? Clearly, since $P^{(2)}$ appears in the evolution equation for $P^{(1)}$, we must investigate the time evolution for $P^{(2)}$; now, as is clear, the evolution equation for $P^{(2)}$ contains another function, $P^{(3)}$, which depends on time and the coordinates and velocities of three molecules and gives the probability density of finding, at time t, the first molecule at $\mathbf{x}_1$ with velocity $\boldsymbol{\xi}_1$, the second at $\mathbf{x}_2$ with velocity $\boldsymbol{\xi}_2$ and the third at $\mathbf{x}_3$ with velocity $\boldsymbol{\xi}_3$. In general if we introduce a function $P^{(s)} = P^{(s)}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_s, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_s, t)$, the so-called *s-particle distribution function*, which gives the probability density of finding, at time t, the first molecule at $\mathbf{x}_1$ with velocity $\boldsymbol{\xi}_1$, the second at $\mathbf{x}_2$ with velocity $\boldsymbol{\xi}_2, \ldots$and the s-th at $\mathbf{x}_s$ with velocity $\boldsymbol{\xi}_s$, we find the evolution equation of $P^{(s)}$ contains the next function $P^{(s+1)}$, till we reach $s = N$; in fact $P^{(N)}$ satisfies a partial differential equation called the Liouville equation. It is clear thus that we cannot proceed unless we handle all the $P^{(s)}$ at the same time and attempt to prove a generalized form of molecular chaos, i.e.,

$$P^{(s)}(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_s, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_s, t) = \prod_{j=1}^{s} P^{(1)}(\mathbf{x}_j, \boldsymbol{\xi}_j, t). \tag{1.2.19}$$

The task then becomes to show that, if true at $t = 0$, this property remains preserved (for any fixed s) in the Boltzmann–Grad limit. This point will be briefly discussed in the next chapter.

There remains the problem of justifying the *initial chaos assumption*, according to which Eq. (1.2.19) is satisfied at $t = 0$. One can give two justifications, one of them being physical in nature and the second mathematical; essentially, they say the same thing, i.e., that it is hard to prepare an initial state for which Eq. (1.2.19) does not hold. The physical reason for this is that, in general, we cannot handle every single molecule, but rather act on the gas as a whole, if we act at a macroscopic level, usually starting from an equilibrium state (for which Eq. (1.2.19) holds). The mathematical argument indicates that if we choose the initial data for the molecules at random, there is an overwhelming probability that Eq. (1.2.19) is satisfied for $t = 0$[7,8].

A word should be said about boundary conditions. When proving that chaos is preserved in the limit, it is absolutely necessary to have a boundary condition compatible (at least in the limit) with Eq. (1.2.19). If the boundary conditions are those of periodicity or specular reflection, no problems arise. More in general, it is sufficient that the particles are scattered without adsorption from the boundary in a way that does not depend on the state of the other molecules of the gas[7,8].

1.3 Molecules Different from Hard Spheres

In the previous section we have discussed the Boltzmann equation when the molecules are assumed to be identical hard spheres. There are several possible generalizations of this molecular model, the most obvious being the case of molecules which are identical point masses interacting with a central force, a good general model for monatomic gases. If the range of the force extends to infinity, there is a complication due to the fact that two molecules are always interacting and the analysis in terms of "collisions" is no longer possible. If, however, the gas is sufficiently dilute, we can take into account that the molecular interaction is negligible for distances larger than a certain σ (the "molecular diameter") and assume that when two molecules are at a distance smaller than σ, then no other molecule is interacting with them and the binary collision analysis considered in the previous section can be applied. The only difference arises in the factor $\sigma^2|(\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1) \cdot \mathbf{n}|$ which turns out to be replaced by a function of $V = |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|$ and the angle θ between $\mathbf{n}$ and $\mathbf{V}$.[7,8] Thus the Boltzmann equation for monatomic molecules takes on the following form:

$$\frac{\partial P^{(1)}}{\partial t} + \boldsymbol{\xi}_1 \cdot \frac{\partial P^{(1)}}{\partial \mathbf{x}_1} = N \int_{R^3} \int_{\mathcal{B}_-} [P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1', t) P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2', t)$$

$$-P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_1, t) P^{(1)}(\mathbf{x}_1, \boldsymbol{\xi}_2, t)] B(\theta, |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|) d\boldsymbol{\xi}_2 d\theta d\epsilon \tag{1.3.1}$$

where ϵ is the other angle which, together with θ, identifies the unit vector $\mathbf{n}$. The function $B(\theta, V)$ depends, of course, on the specific law of interaction between the molecules. In the case of hard spheres, of course

$$B(\theta, |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|) = \cos\theta \sin\theta |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|. \tag{1.3.2}$$

In spite of the fact that the force is cut at a finite range σ when writing the Boltzmann equation, infinite range forces are frequently used. This has the disadvantage of making the integral in Eq. (1.3.1) rather hard to handle; in fact, one cannot split it into the difference of two terms (the loss and the gain), because each of them would be a divergent integral. This disadvantage is compensated in the case of power law forces, because one can separate the dependence on θ from the dependence upon $|\mathbf{V}|$. In fact, one can show[7,8] that, if the intermolecular force varies as the n-th inverse power of the distance, then

$$B(\theta, |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|) = \beta(\theta) |\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1|^{\frac{n-5}{n-1}} \tag{1.3.3}$$

where $\beta(\theta)$ is a non-elementary function of θ (in the simplest cases it can be expressed by means of elliptic functions). In particular, for $n = 5$ one has the so-called Maxwell molecules, for which the dependence on V disappears.

Sometimes the artifice of cutting the grazing collisions corresponding to small values of $|\theta - \frac{\pi}{2}|$ is used (angle cutoff). In this case one has both the advantage of being able to split the collision term and of preserving a relation of the form (1.3.3) for power-law potentials.

Since solving the Boltzmann equation with actual cross sections is complicated, in many numerical simulations use is made of the so-called variable hard sphere (VHS) model in which the diameter of the spheres is an inverse power law function of the relative speed $|\mathbf{V}|$.

Another important case is when we deal with a mixture rather than with a single gas. In this case we have n unknowns, if n is the number of the species, and n Boltzmann equations; in each of them there are n collision terms to describe the collision of a molecule with other molecules of all the possible species[7].

If the gas is polyatomic, then the gas molecules have other degrees of freedom in addition to the translation ones. This in principle requires using quantum mechanics, but one can devise useful and accurate models in the classical scheme as well. Frequently the internal energy E_i is the only additional variable that is needed; in which case one can think of the gas as of a mixture of species[7], each differing from the other because of the value of E_i. If the latter variable is discrete we obtain a strict analogy with a mixture; otherwise we have a continuum of species. We remark that in both cases, kinetic energy is not preserved by collisions, because internal energy also enters into the balance; this means that a molecule changes its "species" when colliding. This is the simplest example of a "reacting collision", which may be generalized to actual chemical species when chemical reactions occur.

1.4 Collision Invariants

Before embarking a discussion of the properties of the solutions of the Boltzmann equation we remark that the unknown of the latter is not always chosen to be a probability density as we have done so far; it may be multiplied by a suitable factor and transformed into an (expected) number density or an (expected) mass density (in phase space, of course). The only thing that changes is the factor in front of Eq. (1.3.1) which is no longer N. In order to avoid any commitment to a special choice of that factor we replace $NB(\theta, V)$ by $\mathcal{B}(\theta, V)$ and the unknown P by another letter, f (which is also the most commonly used letter to denote the one-particle distribution function, no matter what its normalization is). In addition, we replace the current velocity variable $\boldsymbol{\xi}_1$ simply by $\boldsymbol{\xi}$ and $\boldsymbol{\xi}_2$ by $\boldsymbol{\xi}_*$. Thus we rewrite Eq. (1.3.1) in the following form:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = \int_{R^3} \int_{\mathcal{B}^-} (f' f'_* - f f_*) \mathcal{B}(\theta, V) d\boldsymbol{\xi}_* d\theta d\epsilon \tag{1.4.1}$$

where $V = |\boldsymbol{\xi} - \boldsymbol{\xi}_*|$. The velocity arguments $\boldsymbol{\xi}'$ and $\boldsymbol{\xi}'_*$ in f' and f'_* are of course given by Eqs. (1.2.1) (or (1.2.16)) with the suitable modification.

The right-hand side of Eq. (1.4.1) contains a quadratic expression $Q(f, f)$, given by

$$Q(f,f) = \int_{R^3}\int_{S^2}(f'f'_* - ff_*)\mathcal{B}(\theta,V)d\boldsymbol{\xi}_*d\theta d\epsilon. \tag{1.4.2}$$

This expression is called the collision integral or, simply, the collision term and the quadratic operator Q goes under the name of collision operator. In this section we study some elementary properties of Q. Actually it turns out that it is more convenient to study the slightly more general bilinear expression associated with $Q(f,f)$, i.e.:

$$Q(f,g) = \frac{1}{2}\int_{R^3}\int_{S^2}(f'g'_* + g'f_* - fg_* - gf_*)\mathcal{B}(\theta,V)d\boldsymbol{\xi}_*d\theta d\epsilon. \tag{1.4.3}$$

It is clear that when $g = f$, Eq. (1.4.3) reduces to Eq. (1.4.2) and

$$Q(f,g) = Q(g,f). \tag{1.4.4}$$

Our first aim is to study the eightfold integral:

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}_-}(f'g'_* + g'f'_* - fg_* - gf_*)\phi(\boldsymbol{\xi})\mathcal{B}(\theta,V)d\boldsymbol{\xi}_*d\boldsymbol{\xi}d\theta d\epsilon \tag{1.4.5}$$

where f, g and ϕ are functions such that the indicated integrals exist and the order of integration does not matter. A simple interchange of the starred and unstarred variables (with a glance at Eqs. (1.2.1)) shows that

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}_-}(f'g'_* + g'f'_* - fg_* - gf_*)\phi(\boldsymbol{\xi}_*)\mathcal{B}(\theta,V)d\boldsymbol{\xi}_*d\boldsymbol{\xi}d\theta d\epsilon. \tag{1.4.6}$$

Next, we consider another transformation of variables, the exchange of primed and unprimed variables (which is possible because the transformation in Eq. (1.2.1) is linear and its own inverse, for any fixed $\mathbf{n}$). This gives

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}^-}(fg_* + gf_* - f'g'_* - g'f_*)\phi(\boldsymbol{\xi}')\mathcal{B}(\theta,V)d\boldsymbol{\xi}'_*d\boldsymbol{\xi}'d\theta d\epsilon. \tag{1.4.7}$$

(Actually since $\mathbf{V}'\cdot\mathbf{n} = -\mathbf{V}\cdot\mathbf{n}$ we should write $\mathcal{B}^-$ in place of B^+; changing $\mathbf{n}$ into $-\mathbf{n}$, however, gives exactly the expression written here.)

The absolute value of the Jacobian from $\boldsymbol{\xi}, \boldsymbol{\xi}_*$ to $\boldsymbol{\xi}', \boldsymbol{\xi}'_*$ is unity; thus we can write $d\boldsymbol{\xi} d\boldsymbol{\xi}_*$ in place of $d\boldsymbol{\xi}' d\boldsymbol{\xi}'_*$ and Eq. (1.4.7) becomes:

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}-} (fg_* + gf_* - f'g'_* - g'f'_*)\phi(\boldsymbol{\xi}')\mathcal{B}(\theta, V)d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\theta d\epsilon. \tag{1.4.8}$$

Finally we can interchange the starred and unstarred variables in Eq. (1.4.8) to find:

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}-} (fg_* + gf_* - f'g'_* - g'f'_*)\phi(\boldsymbol{\xi}'_*)\mathcal{B}(\theta, V)d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\theta d\epsilon. \tag{1.4.9}$$

Eqs. (1.4.6), (1.4.8), (1.4.9) differ from Eq. (1.4.5) because the factor $\phi(\boldsymbol{\xi})$ is replaced by $\phi(\boldsymbol{\xi}_*)$, $-\phi(\boldsymbol{\xi}')$ and $-\phi(\boldsymbol{\xi}_*)$ respectively. We can now obtain more expressions for the integral in the left-hand side by taking linear combinations of the four different expressions available. Among them, the most interesting one is the symmetric expression obtained by taking the sum of Eqs. (1.4.5), (1.4.6), (1.4.8), (1.4.9) and dividing by four. The result is:

$$\int_{R^3} Q(f,g)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{8}\int_{R^3}\int_{R^3}\int_{\mathcal{B}-} (f'g'_* + g'f'_* - fg_* - gf_*)(\phi + \phi_* - \phi' - \phi'_*)\mathcal{B}(\theta, V)d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\theta d\epsilon. \tag{1.4.10}$$

This relation expresses a basic property of the collision term, which is frequently used. In particular, when $g = f$, Eq. (1.4.10) reads

$$\int_{R^3} Q(f,f)\phi(\boldsymbol{\xi})d\boldsymbol{\xi}$$

$$= \frac{1}{4}\int_{R^3}\int_{R^3}\int_{\mathcal{B}-} (f'f'_* - ff_*)(\phi + \phi_* - \phi' - \phi'_*)\mathcal{B}(\theta, V)|d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\theta d\epsilon. \tag{1.4.11}$$

We remark that the following form also holds:

$$\int_{R^3} Q(f,f)\phi(\boldsymbol{\xi})d\boldsymbol{\xi} = \frac{1}{2}\int_{R^3}\int_{R^3}\int_{\mathcal{B}_-} ff_*(\phi' + \phi'_* - \phi - \phi_*)\mathcal{B}(\theta, V)d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\theta d\epsilon. \tag{1.4.12}$$

In fact, the integral in Eq. (1.4.11) can be split into the difference of two integrals (one containing $f'f'_*$, the other ff_*); the two integrals are just the opposite of each other, as an exchange between primed and unprimed variables shows, and Eq. (1.4.12) holds.

We now observe that the integral in Eq. (1.4.10) is zero independent of the particular functions f and g, if

$$\phi + \phi_* = \phi' + \phi'_* \tag{1.4.13}$$

is valid almost everywhere in velocity space. Since the integral appearing in the left-hand side of Eq. (1.4.11) is the rate of change of the average value of the function ϕ due to collisions, the functions satisfying Eq. (1.4.13) are called "collision invariants". It can be easily shown that a continuous function ϕ has the property expressed by Eq. (1.4.13) if and only if

$$\phi(\boldsymbol{\xi}) = a + \mathbf{b}\cdot\boldsymbol{\xi} + c|\boldsymbol{\xi}|^2 \tag{1.4.14}$$

where a and c are constant scalars and $\mathbf{b}$ a constant vector. The assumption of continuity can be considerably relaxed[2,3,10]. The functions $\psi_0 = 1, (\psi_1, \psi_2, \psi_3) = \boldsymbol{\xi}, \psi_4 = |\boldsymbol{\xi}|^2$ are usually called the elementary collision invariants; they span the five-dimensional subspace of the collision invariants.

Thus, summarizing, a collision invariant is a function ϕ such that

$$\int_{R^3} \phi(\boldsymbol{\xi}) Q(f,g) d\boldsymbol{\xi} = 0, \tag{1.4.15}$$

and the most general expression of a collision invariant is given by Eq. (1.4.14).

1.5 The Boltzmann Inequality and the Maxwell Distributions

In this section we investigate the existence of positive functions f which give a vanishing collision integral:

$$Q(f,f) = \int_{R^3} \int_{\mathcal{B}^-} (f'f'_* - ff_*)\mathcal{B}(\theta, V) d\boldsymbol{\xi}_* d\theta d\epsilon = 0. \tag{1.5.1}$$

In order to solve this equation, we prove a preliminary result which plays an important role in the theory of the Boltzmann equation: if f is a nonnegative function such that $\log f\, Q(f,f)$ is integrable and the manipulations of the previous section hold when $\phi = \log f$, then the *Boltzmann inequality*

$$\int_{R^3} \log f\, Q(f,f) d\boldsymbol{\xi} \leq 0 \tag{1.5.2}$$

holds; further, the equality sign applies if, and only if, $\log f$ is a collision invariant, or, equivalently,

$$f = \exp(a + \mathbf{b}\cdot\boldsymbol{\xi} + c|\boldsymbol{\xi}|^2). \tag{1.5.3}$$

To prove Eq. (1.5.2) it is enough to use Eq. (1.4.11) with $\phi = \log f$:

$$\int_{R^3} \log f\, Q(f,f) d\boldsymbol{\xi} = \frac{1}{4} \int_{R^3} \int_{\mathcal{B}^-} \log(f f_* / f' f'_*)(f' f'_* - f f_*) \mathcal{B}(\theta, V) d\boldsymbol{\xi} d\boldsymbol{\xi}_* d\epsilon \tag{1.5.4}$$

and Eq. (1.5.2) follows thanks to the elementary inequality

$$(z-y)\log(y/z) \leq 0 \quad (y, z \in R^+). \tag{1.5.5}$$

Eq. (1.5.5) becomes an equality if and only if $y = z$; thus the equality sign holds in Eq. (1.5.2) if and only if

$$f' f'_* = f f_* \tag{1.5.6}$$

applies almost everywhere. But, taking the logarithms of both sides of Eq. (1.5.6), we find that $\phi = \log f$ satisfies Eq. (1.4.13) and is thus given by Eq. (1.4.14). $f = \exp(\phi)$ is then given by Eq. (1.5.3).

We remark that in the latter equation c must be negative, since f must be integrable. If we let $c = -\beta, \mathbf{b} = 2\beta\mathbf{v}$ (where $\mathbf{v}$ is another constant vector) Eq. (1.5.3) can be rewritten as

$$f = A\exp(-\beta|\boldsymbol{\xi} - \mathbf{v}|^2) \tag{1.5.7}$$

where A is a positive constant related to $a, c, |\,\mathbf{b}\,|^2$ ($\beta, \mathbf{v}, A$ constitute a new set of constants). The function appearing in Eq. (1.2.7) is the so-called *Maxwell distribution* or *Maxwellians*. Frequently one considers Maxwellians with $\mathbf{v} = 0$ (nondrifting Maxwellians), which can be obtained from drifting Maxwellians by a change of the origin in velocity space.

Let us return now to the problem of solving Eq. (1.5.1). Multiplying both sides by $\log f$ gives Eq. (1.5.2) with the equality sign. This implies that f is a Maxwellian, by the result which has just been proved. Suppose now that f is a Maxwellian; then $f = \exp(\phi)$ where ϕ is a collision invariant and Eq. (1.5.6) holds; Eq. (1.5.1) then also holds. Thus there are functions which satisfy Eq. (1.5.1) and they are all Maxwellians, Eq. (1.5.7).

1.6 The Macroscopic Balance Equations

In this section we compare the microscopic description supplied by kinetic theory with the macroscopic description supplied by continuum gas dynamics. For definiteness, in this section f will be assumed to be an expected mass density in phase space. In order to obtain a density $\rho = \rho(x,t)$ in ordinary space, we must integrate f with respect to $\boldsymbol{\xi}$:

$$\rho = \int_{R^3} f d\boldsymbol{\xi}. \tag{1.6.1}$$

The bulk velocity $\mathbf{v}$ of the gas (e.g., the velocity of a wind), is the average of the molecular velocities $\boldsymbol{\xi}$ at a certain point $\mathbf{x}$ and time instant t; since f is proportional to the probability for a molecule to have a given velocity, $\mathbf{v}$ is given by

$$\mathbf{v} = \frac{\int_{R^3} \boldsymbol{\xi} f d\boldsymbol{\xi}}{\int_{R^3} f d\boldsymbol{\xi}} \tag{1.6.2}$$

(the denominator is required even if f is taken to be a probability density in phase space, because we are considering a conditional probability, referring to the position $\mathbf{x}$). Eq. (1.6.2) can also be written as

$$\rho\mathbf{v} = \int_{R^3} \boldsymbol{\xi} f d\boldsymbol{\xi} \tag{1.6.3}$$

or, using components,

$$\rho v_i = \int_{R^3} \xi_i f d\boldsymbol{\xi} \qquad (i = 1, 2, 3). \tag{1.6.4}$$

The bulk velocity $\mathbf{v}$ is what we can directly perceive of the molecular motion by means of macroscopic observations; it is zero for a gas in equilibrium in a box at rest. Each molecule has its own velocity $\boldsymbol{\xi}$ which can be decomposed into the sum of $\mathbf{v}$ and another velocity

$$\mathbf{c} = \boldsymbol{\xi} - \mathbf{v} \tag{1.6.5}$$

called the random or peculiar velocity; $\mathbf{c}$ is clearly due to the deviations of $\boldsymbol{\xi}$ from $\mathbf{v}$. It is also clear that the average of $\mathbf{c}$ is zero.

The quantity ρv_i which appears in Eq. (1.6.4) is the i-th component of the mass flow or, alternatively, of the momentum density of the gas. Other quantities of similar nature are: the momentum flow

$$m_{ij} = \int_{R^3} \xi_i \xi_j f d\boldsymbol{\xi} \qquad (i, j = 1, 2, 3)\,; \tag{1.6.6}$$

the energy density per unit volume:

$$w = \frac{1}{2}\int_{R^3} |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi}\,; \tag{1.6.7}$$

the energy flow:

$$r_i = \frac{1}{2}\int_{R^3} \xi_i |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi} \qquad (i, j = 1, 2, 3)\,. \tag{1.6.8}$$

Eq. (1.6.8) shows that the momentum flow is described by the components of a symmetric tensor of second order, because we must describe the flow in the i-th direction of the j-th component of momentum. It is to be expected that in a macroscopic description only a part of this tensor will be identified as a bulk momentum flow, because, in general, m_{ij} will be different from zero even in the absence of a macroscopic motion ($\mathbf{v} = 0$). It is thus convenient to re-express the integral in m_{ij} in terms of $\mathbf{c}$ and $\mathbf{v}$. Then we have:

$$m_{ij} = \rho v_i v_j + p_{ij} \tag{1.6.9}$$

where

$$p_{ij} = \int_{R^3} c_i c_j f d\boldsymbol{\xi}; \qquad (i, j = 1, 2, 3) \tag{1.6.10}$$

plays the role of the stress tensor (because the microscopic momentum flow associated with it is equivalent to forces distributed on the boundary of any region of gas, according to the macroscopic description).

Similarly one has

$$w = \frac{1}{2}\rho|\mathbf{v}|^2 + \rho e, \tag{1.6.11}$$

where e is the internal energy per unit mass (associated with random motions) defined by

$$\rho e = \frac{1}{2}\int_{R^3} |\mathbf{c}|^2 f d\boldsymbol{\xi} \tag{1.6.12}$$

and

$$r_i = \rho v_i (\frac{1}{2}|\mathbf{v}|^2 + e) + \sum_{j=1}^{3} v_j p_{ij} + q_i \qquad (i = 1, 2, 3)\,, \tag{1.6.13}$$

where q_i are the components of the so-called heat flow vector:

$$q_i = \frac{1}{2}\int_3 c_i |\mathbf{c}|^2 f d\boldsymbol{\xi}\,. \tag{1.6.14}$$

The decomposition in Eq. (1.6.13) shows that the microscopic energy flow is a sum of a macroscopic flow of energy (both kinetic and internal), of the work (per unit area and unit time) done by stresses, and of the heat flow.

In order to complete the connection, as a simple mathematical consequence of the Boltzmann equation, one can derive five differential relations satisfied by the macroscopic quantities introduced above; these relations describe the balance of mass, momentum and energy and have the same form as in continuum mechanics. To this end let us consider the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f). \tag{1.6.15}$$

If we multiply both sides by one of the elementary collision invariants ψ_α ($\alpha = 0, 1, 2, 3, 4$), defined in Section 4, and integrate with respect to $\boldsymbol{\xi}$, we have, thanks to Eq. (1.4.15) with $g = f$ and $\phi = \psi_\alpha$:

$$\int_{R^3} \psi_\alpha(\boldsymbol{\xi}) Q(f, f) d\boldsymbol{\xi} = 0, \tag{1.6.16}$$

and hence, if it is permitted to change the order by which we differentiate with respect to t and integrate with respect to $\boldsymbol{\xi}$:

$$\frac{\partial}{\partial t}\int \psi_\alpha f d\boldsymbol{\xi} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\int \xi_i \psi_\alpha f d\boldsymbol{\xi} = 0 \qquad (\alpha = 1, 2, 3, 4). \tag{1.6.17}$$

If we take successively $\alpha = 0, 1, 2, 3, 4$ and use the definitions introduced above, we obtain

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho v_i) = 0, \tag{1.6.18}$$

$$\frac{\partial}{\partial t}(\rho v_j) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho v_i v_j + p_{ij}) = 0, \qquad (j = 1, 2, 3) \tag{1.6.19}$$

$$\frac{\partial}{\partial t}(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho e) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left[\rho v_i(\frac{1}{2}|\mathbf{v}|^2 + e) + \sum_{j=1}^{3} v_j p_{ij} + q_i\right] = 0. \tag{1.6.20}$$

These equations have the so-called conservation form because they express the circumstance that a certain quantity (whose density appears differentiated with respect to time) is created or destroyed in a certain region Ω because something is flowing through the boundary $\partial\Omega$. In fact, when integrating both sides of the equations with respect to $\mathbf{x}$ over Ω, the terms differentiated with respect to the space coordinates can be replaced by surface integrals over $\partial\Omega$, thanks to the divergence theorem. If these surface integrals turn out to be zero, then we obtain that the total mass

$$M = \int_\Omega \rho d\mathbf{x}, \tag{1.6.21}$$

the total momentum

$$\mathbf{Q} = \int_{\boldsymbol{\Omega}} \rho \mathbf{v} d\mathbf{x}, \tag{1.6.22}$$

and the total energy

$$E = \int_\Omega (\frac{1}{2}\rho|\mathbf{v}|^2 + \rho e) d\mathbf{x} \ , \tag{1.6.23}$$

are conserved in Ω. Typical cases when this occurs are:

a) Ω is R^3 and suitable conditions at infinity insure that the fluxes of the mass, momentum and energy flow vectors through a large sphere vanish when the radius of the sphere tends to infinity;

b) Ω is a box with periodicity conditions, because essentially there are no boundaries.

When Ω is a compact domain with the condition of specular reflection on Ω, then the boundary terms on $\partial\Omega$ disappear in the mass and energy equations but not in the momentum equation; thus only M and E are conserved.

We also remark that in the so-called space-homogeneous case, the various quantities do not depend on $\mathbf{x}$; all the space derivatives then disappear from Eqs. (1.6.18–20) and the densities $\rho, \rho\mathbf{v}$ and $\frac{1}{2}\rho\,|\,\mathbf{v}\,|^2 + \rho e$ are conserved, i.e. do not change with time.

The considerations of this section apply to all the solutions of the Boltzmann equation. The definitions, however, can be applied to any positive function for which they make sense. In particular if we take f to be a Maxwellian in the form

(1.5.7), we find that the constant vector $\mathbf{v}$ appearing there is actually the bulk velocity as defined in Eq. (1.6.2) while β and A are related to the internal energy e and the density ρ in the following way:

$$\beta = 3/(4e), \qquad A = \rho(4\pi e/3)^{-3/2}. \tag{1.6.24}$$

Furthermore the stress tensor turns out to be diagonal ($p_{ij} = (\frac{2}{3}\rho e)\delta_{ij}$, where δ_{ij} is the "Kronecker delta" (=1 if $i = j; = 0$ if $i \neq j$)), while the heat flow vector is zero.

We end this section with the definition of pressure p in terms of f; p is nothing else than 1/3 of the spur or trace (i.e., the sum of the three diagonal terms) of p_{ij} and is thus given by

$$p = \frac{1}{3}\int_{R^3} |\mathbf{c}|^2 f d\boldsymbol{\xi}. \tag{1.6.25}$$

If we compare this with the definition of the specific internal energy e, given in Eq. (1.6.12), we obtain the relation

$$p = \frac{2}{3}\rho e. \tag{1.6.26}$$

This relation also suggests the definition of temperature, according to kinetic theory, $T = (\frac{2}{3}e)/R$, where R is the gas constant equal to the universal Boltzmann constant k divided by the molecular mass m. Thus

$$T = \frac{1}{3\rho R}\int_{R^3} |\mathbf{c}|^2 f d\boldsymbol{\xi}. \tag{1.6.27}$$

This definition is appropriate, because if we mix two different gases and let them achieve a state of equilibrium, T turns out to be the same for the two gases (see Ref. 7). Thus, if we take into account Eq. (1.6.24), a Maxwellian distribution (see Eq. (1.5.7)) can be written as

$$f = \rho(2\pi RT)^{-3/2}\exp[-|\boldsymbol{\xi} - \mathbf{v}|^2/(2RT)]. \tag{1.6.28}$$

1.7 The H-theorem

Let us consider a further application of the properties of the collision term $Q(f, f)$ of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{x}} = Q(f, f). \tag{1.7.1}$$

If we multiply both sides of this equation by $\log f$ and integrate with respect to $\boldsymbol{\xi}$, we obtain

$$\frac{\partial \mathcal{H}}{\partial t} + \frac{\partial}{\partial \mathbf{x}}\cdot\mathbf{J} = \mathcal{S} \tag{1.7.2}$$

where

$$\mathcal{H} = \int_{R^3} f \log f d\boldsymbol{\xi}, \tag{1.7.3}$$

$$\mathbf{J} = \int_{R^3} \boldsymbol{\xi} f \log f d\boldsymbol{\xi}, \tag{1.7.4}$$

$$\mathcal{S} = \int_{R^3} \log f \, Q(f,f) d\boldsymbol{\xi}. \tag{1.7.5}$$

Eq. (1.7.2) differs from the balance equations considered in the previous section because the right side, generally speaking, does not vanish. We know, however, that the Boltzmann inequality, Eq. (1.5.2), implies:

$$\mathcal{S} \leq 0 \quad \text{and} \quad \mathcal{S} = 0 \quad \text{iff} \quad f \text{ is a Maxwellian.} \tag{1.7.6}$$

Because of this inequality, Eq. (1.7.2) plays an important role in the theory of the Boltzmann equation. We illustrate the role of Eq. (1.7.6) in the case of space-homogeneous solutions. In this case the various quantities do not depend on $\mathbf{x}$ and Eq. (1.7.2) reduces to

$$\frac{\partial \mathcal{H}}{\partial t} = \mathcal{S} \leq 0. \tag{1.7.7}$$

This implies the so-called H-theorem (for the space homogeneous case): $\mathcal{H}$ is a decreasing quantity, unless f is a Maxwellian (in which case the time derivative of $\mathcal{H}$ is zero). Remember now that in this case the densities $\rho, \rho\mathbf{v}$ and ρe are constant in time; we can thus build a Maxwellian M which has, at any time, the same $\rho, \mathbf{v}$ and e as any solution f corresponding to given initial data. Since $\mathcal{H}$ decreases unless f is a Maxwellian (i.e., $f = M$), it is tempting to conclude that f tends to M when $t \to \infty$. The temptation is strengthened when we realize that $\mathcal{H}$ is bounded from below by $\mathcal{H}_M$, the value taken by the functional $\mathcal{H}$ when $f = M$. In fact $\mathcal{H}$ is decreasing, its derivative is nonpositive unless it takes the value $\mathcal{H}_M$; one feels that $\mathcal{H}$ tends to $\mathcal{H}_M$! This conclusion is, however, unwarranted from a purely mathematical viewpoint, without a more detailed consideration of the source term $\mathcal{S}$ in Eq. (1.7.7). If the state of the gas is not space-homogeneous, the situation becomes more complicated. In this case it is convenient to introduce the quantity

$$H = \int_{\Omega} \mathcal{H} d\mathbf{x} \tag{1.7.8}$$

where Ω is the space domain occupied by the gas (assumed here to be time-independent). Then Eq. (1.7.2) implies

$$\frac{dH}{dt} \leq \int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} d\sigma \tag{1.7.9}$$

where $\mathbf{n}$ is the inward normal and $d\sigma$ the surface element on $\partial\Omega$. Clearly, several situations may arise. Among the most typical ones, we quote:

1. Ω is a box with periodicity boundary conditions (flat torus). Then there is no boundary, $dH/dt \leq 0$ and one can repeat about H what was said about $\mathcal{H}$ in the space-homogeneous case. In particular, there is a natural (space-homogeneous) Maxwellian associated with the total mass, momentum and energy (which are conserved as was remarked in the previous section).

2. Ω is a compact domain with specular reflection. In this case the boundary term also disappears because the integrand of $\mathbf{J} \cdot \mathbf{n}$ is odd on $\partial\Omega$ and the situation is similar to that in case 1. There might seem to be a difficulty for the choice of the natural Maxwellian because momentum is not conserved, but a simple argument shows that the total momentum must vanish when $t \to \infty$. Thus M is a non-drifting Maxwellian.

3. Ω is the entire space. Then the asymptotic behavior of the initial values at ∞ is of paramount importance. If the gas is initially more concentrated at finite distances from the origin, one physically expects that the gas escapes through infinity and the asymptotic state is a vacuum.

4. Ω is a compact domain but the boundary conditions on $\partial\Omega$ are different from specular reflection. Then the asymptotic state may be completely different from a Maxwellian because the gas may be forced to remain in a non-equilibrium state.

Boltzmann's H-theorem is of basic importance because it shows that his equation has a basic feature of irreversibility: the quantities $\mathcal{H}$ (in the space-homogeneous case) and H (in other cases where the gas does not exchange mass and energy with a solid boundary) always decrease in time. This result seems to be in conflict with the fact that the molecules constituting the gas follow the laws of classical mechanics which are time reversible, but there is a way out of this paradox[11]. It should be clear that H has the properties of entropy (except for the sign); this identification is strengthened when we evaluate H in an equilibrium state because it turns out to coincide with the expression of a perfect gas according to equilibrium thermodynamics, apart from a factor $-R$. A further check of this identification is given by an inequality satisfied by the right-hand side of Eq. (1.7.9) when the gas is able to exchange energy with a solid wall bounding Ω (see Chapter 4).

1.8 Equilibrium States and Maxwellian Distributions

The trend toward a Maxwellian distribution expressed by the H-theorem indicates that this particular distribution is a good candidate to describe a gas in a (statistical) equilibrium state. In order to prove that Maxwellians describe the equilibrium states of a gas, however, we must give a definition of equilibrium. Intuitively, a gas is in equilibrium if, in a situation where it does not exchange mass and energy with other bodies, its state does not change with time. Thus for the moment we define an equilibrium state to be one of a gas in a steady situation in a box with periodicity or specular reflection boundary conditions. It is then clear that the distribution function must be a Maxwellian; in fact, Eq. (1.7.2) implies (when $\mathcal{H}$ does not depend on time):

$$\int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} d\sigma = \int_{\Omega} \mathcal{S} d\mathbf{x} \leq 0 \tag{1.8.1}$$

where $\mathbf{n}$ is the inward normal and equality holds if and only if f is Maxwellian. But $\mathbf{J} \cdot \mathbf{n}$ is zero for the situation under consideration and the only possibility is that f be a Maxwellian. We impose now the condition that this Maxwellian must be a steady solution of the Boltzmann equation i.e., must satisfy

$$\boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f)\,. \tag{1.8.2}$$

This readily implies that both the right- and the left-hand side of the Boltzmann equation must vanish ; as a consequence, the parameters A, β and $\mathbf{v}$ appearing in the Maxwellian

$$f = A \exp(-\beta |\boldsymbol{\xi} - \mathbf{v}|^2) \tag{1.8.3}$$

must be of the form $\mathbf{v} = \mathbf{v}_0 + \boldsymbol{\omega} \wedge \mathbf{x}$, $A = A_0 \exp[|\boldsymbol{\omega}|^2 \,|\,\mathbf{x}\,|^2 - (\boldsymbol{\omega} \cdot \mathbf{x})^2]$, $\beta =$constant (where $\mathbf{v}_0$ and $\boldsymbol{\omega}$ are constant vectors, A_0 a constant scalar, and $\wedge$ denotes the vector product). If the periodicity condition in a box or the specular reflection boundary condition (in a general domain not rotationally invariant about the direction of $\boldsymbol{\omega}$) is imposed, it turns out that also A and $\mathbf{v}$ must be constant (and not space dependent). Thus, in general, a Maxwellian with constant parameters is the most general equilibrium solution of the Boltzmann equation.

The question immediately arises, whether there are solutions of the Boltzmann equation which are Maxwellians with parameters depending on $\mathbf{x}$ and t. Since the right hand side of the Boltzmann equation vanishes identically if f is a Maxwellian, it turns out that a Maxwellian, i.e., a function of the form specified in Eq. (1.8.3), can be a solution of the Boltzmann equation if, and only if, A, β and $\mathbf{v}$ depend on t and $\mathbf{x}$ in such a way that f also satisfies

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = 0. \tag{1.8.4}$$

Since the general solution of this equation has the form $f = f(\mathbf{x} - \boldsymbol{\xi} t, \mathbf{x} \wedge \boldsymbol{\xi}, \boldsymbol{\xi})$, it turns out that there are several solutions of this form; they were investigated by Boltzmann in 1876. Among them we quote the case met above in which $\mathbf{v} = \mathbf{v}_0 + \boldsymbol{\omega} \wedge \mathbf{x}$, $A = A_0 \exp[|\boldsymbol{\omega}|^2 \,|\,\mathbf{x}\,|^2 - (\boldsymbol{\omega} \cdot \mathbf{x})^2]$, $\beta =$constant (with $\mathbf{v}_0$, A_0 and $\boldsymbol{\omega}$ constants) and the case in which $A =$constant, $\beta = \beta_0(1 + t/t_0)^2$, $\mathbf{v} = (t + t_0)^{-1}\mathbf{x}$. The latter solution describes a compression if t_0 is negative (but the solution ceases to exist for $t > |t_0|$), and an expansion into a vacuum if $t_0 > 0$ (in which case the solution exists for any positive time).

1.9 The Boltzmann Equation in General Coordinates

It is, of course, easy to write the Boltzmann equation using the Cartesian components x_i and $\boldsymbol{\xi}_i$ (i=1,2,3) of the vectors $\mathbf{x}$ and $\boldsymbol{\xi}$. It is more complicated to write the left-hand side when more general coordinates such as cylindrical or spherical are used. It is not enough to take the components of $\boldsymbol{\xi}$ and $\partial f/\partial \mathbf{x}$ and form their scalar product. In fact, f is a function of both $\mathbf{x}$ and $\boldsymbol{\xi}$ and one should take this into account. Let us denote by q^i $(i = 1, 2, 3)$ the i-th coordinate and by $p^i = \dot{q}^i$ $(i = 1, 2, 3)$ its time derivative. In general coordinates, we must distinguish between covariant and contravariant components. The metric form is easily provided by the kinetic energy per unit mass K expressed in terms of q^i and p^i. We have then

$$p_i = \frac{\partial K}{\partial p^i}.$$

The metric tensor is given by

$$a_{ik} = \frac{\partial^2 K}{\partial p^i \partial p^k}$$

and the related a^{ik} are such that $a_{ij}a^{jk} = \delta_i^k$. Because of Lagrange's equations for inertial motion,

$$\dot{p}_i = \frac{\partial K}{\partial q^i}.$$

Then $f = f(q^i, p_i, t)$ and

$$\boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = p^i \frac{\partial f}{\partial q^i} + \frac{\partial K}{\partial q^i}\frac{\partial f}{\partial p_i}$$

where the sum convention is adopted.

Let us consider, as an example, the case of cylindrical coordinates (r, φ, z). The p^i are now (ξ_r, ω, ξ_z) where $\omega = \xi_\varphi / r$ and $K = \frac{1}{2}((\xi_r)^2 + (r\omega)^2 + (\xi_z)^2$. As a consequence, the p_i's are $(\xi_r, p_\varphi, \xi_z)$ where $p_\varphi = r^2\omega = r\xi_\varphi$. In conclusion, we have

$$\boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = \xi_r \frac{\partial f}{\partial r} + \xi_\varphi \frac{\partial f}{\partial \varphi} + \xi_z \frac{\partial f}{\partial z} + \frac{(\xi_\varphi)^2}{r}\frac{\partial f}{\partial \xi_r}.$$

One must be careful, however, because the partial derivatives are computed for $f = f((r, \varphi, z, \xi_r, p_\varphi, \xi_z)$ and not for $f = f((r, \varphi, z, \xi_r, \xi_\varphi, \xi_z)$ as is sometimes more natural. If the latter variables are chosen, then

$$\dot{\xi}_r = \frac{(\xi_\varphi)^2}{r}; \quad \dot{p}_\varphi = 0$$

are replaced by

$$\dot{\xi}_r = \frac{(\xi_\varphi)^2}{r}; \quad \dot{\xi}_\varphi = -\frac{\xi_r \xi_\varphi}{r}$$

and, as a consequence

$$\boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = \xi_r \frac{\partial f}{\partial r} + \xi_\varphi \frac{\partial f}{\partial \varphi} + \xi_z \frac{\partial f}{\partial z} + \frac{(\xi_\varphi)^2}{r} \frac{\partial f}{\partial \xi_r} - \frac{\xi_r \xi_\varphi}{r} \frac{\partial f}{\partial \xi_\varphi}.$$

1.10 Mean Free Path

Before ending this chapter we briefly discuss the concept of mean free path. The mean free path is the average distance covered by a molecule, i.e., (to simplify) a hard sphere whose diameter we shall denote by σ, between two subsequent collisions. We can consider a moving molecule that strikes any of the other molecules, which are assumed to be motionless (this introduces no essential difference and simplifies the explanation). A collision occurs when the center of the moving sphere comes at a distance equal to σ from the center of a sphere at rest. Then, in order to compute the length of the path between two collisions, we can consider the moving sphere S as a point and the sphere at rest as having a doubled radius, σ (Fig. 1.3). Then if S travels a distance ℓ on average between two impacts, this means that there is only one molecule, i.e., S, in a cylinder of base $\pi\sigma^2$ and height ℓ or $n\pi\sigma^2\ell \cong 1$ where $n = N/V$ is the number of molecules per unit volume. Hence $\ell \cong 1/(n\pi\sigma^2)$. This simple argument shows that ℓ equals $1/(n\pi\sigma^2)$, except for a numerical factor that depends on the way we perform the average implied by the use of the word "mean". For molecules other than hard spheres the concept becomes a little fuzzy although it retains its usefulness as a typical length covered by a molecule between two (significant) interactions. Thus the concept of mean free path is a qualitative one; it can be made precise in several different ways. The different ways produce slightly different values for ℓ; thus it is advisable to check the precise definition adopted by each author, whenever a "mean free path" is spoken of. Whenever we adopt the standard definition in this book (to be given later) we shall use the letter λ rather than ℓ.

Both direct and indirect methods give a value for ℓ (or λ) at room temperature and the atmospheric pressure of about a millionth of a centimeter. The mean free path becomes smaller at lower densities, such as those encountered by an object flying in the upper atmosphere. A gas is called rarefied when the mean free path is not negligible with respect to another typical length; thus, e.g. the air in a street can be considered as a rarefied gas if we are interested in polluting particles having a size of the order of a millionth of a centimeter. Similarly, the air flowing between a disk in a computer and the read/write head is rarefied in this sense, because the distance between the two bodies is of the order of 0.5×10^{-6} centimeters. There are many examples of this kind in modern nanotechnologies; as opposed to space applications of rarefied gas dynamics, the speeds coming into play in all these cases are small compared to the speed of sound, and this explains the interest of the subject of this book, the mathematics of slow rarefied flows.

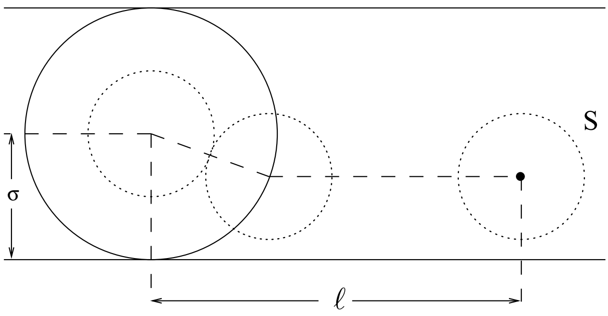

Figure 1.3: The free path of a molecule between two collisions. The moving molecule S is represented as a point, the other molecules as spheres with double radius (the distance between the centers at the point of contact). The dotted circles represent the actual spheres.

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Chapter 2

Validity and Existence

2.1 Introductory Remarks

In Chapter 1 we gave a formal derivation of the Boltzmann equation from the basic laws of mechanics. The objective of this chapter is to indicate how to perform all these steps rigorously, wherever possible. In particular, our discussion will indicate how to reach a rigorous validity result for the Boltzmann equation, locally for a general situation and globally for a rare gas cloud in vacuum, and how to establish an existence theory for this equation.

The importance of the first issue is evident: We have to settle the fundamental question whether the *irreversible* Boltzmann equation can be rigorously obtained from *reversible* mechanics. The answer to this query is yes, as we shall see. In particular, there is no contradiction between the second law of thermodynamics and the reversibility of molecular dynamics, at least for the hard sphere model of a rarefied gas.

We will start, as in Chapter 1, from the hard spheres flow; the latter is only almost everywhere defined. In fact, there is a set of zero measure corresponding to "multiple collisions" (more than two spheres are in contact) where we cannot define the outcome of the collision. In addition, the marginal distribution densities $P^{(s)}$ will only be L^1-functions, no matter how regular they were at time zero. However, the collision term involves restrictions of $P^{(s)}$ to sets of codimension 1, a restriction which does not immediately make sense at this level of regularity. A rigorous derivation of the equations satisfied by the marginals is important, but unfortunately rather technical; we omit it here.

The next and still more difficult step is to take the Boltzmann–Grad limit and prove that the solution of the hierarchy for the marginals converges to a solution of the limiting hierarchy. For short times, this was first done by O. Lanford in a classical paper [6]. Lanford's paper contains only a sketch of the proof; a more detailed treatment is given in two monographs [2,7]. The first of these texts presents also an extension [4,5], due to Illner and Pulvirenti, which gives a global validity result for a gas cloud in all space if the mean free path is large. This is the only global result known so far. In both cases, one can prove propagation of chaos and existence and uniqueness of solutions for the Boltzmann equation.

2.2 Lanford's Theorem

Let $P^{(s)}(\mathbf{z}^s, t)$ be the s-particle distribution function introduced in the previous section. Here, $\mathbf{z}^s = (\mathbf{x}_1, \ldots, \mathbf{x}_s, \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_s)$ is used as a shorthand for the $6s$-dimensional phase point describing the state of the first s particles. We write $\mathbf{z} = (\mathbf{z}^s, \mathbf{z}^{N-s})$, with the obvious meaning of the symbols. In particular $P^{(N)}$ is simply denoted by P and its initial value at time $t = 0$ by P_0. We denote by T^t the operator giving the dynamics of N hard spheres, i.e., $T^t\mathbf{z}$ denotes the position (in the $6N$-dimensional phase space) of the center of a sphere occupying the position $\mathbf{z}$ at time $t = 0$.

We assume that

1. Since the particles are identical, $P_0(\mathbf{z})$ is symmetric with respect to all particles, i.e., for any permutation Π (reordering of the particles) $P_0(\Pi\mathbf{z}) = P_0(\mathbf{z})$. Because $\Pi T^t\mathbf{z} = T^t\Pi\mathbf{z}$, it follows that also $P(\cdot, t)$ has this symmetry.

By Ω^s, $1 \le s \le N$, we denote the phase space of s particles (phase points leading to multiple collisions, etc., are deleted). The time evolution of the s particles of which $P^{(s)}(\mathbf{z}^s, t)$ keeps track is influenced by the interactions of the s particles with the remaining $N - s$ particles. In order to be able to quantify these interactions, we need one further assumption on P_0:

2. We require that $t \to P_0(T^t\mathbf{z})$ is continuous for almost all $\mathbf{z} \in \Omega$.

Assumption 2 deserves a further comment. If $\mathbf{z}$ is an N-particle precollisional phase point and $\mathbf{z}'$ is the corresponding postcollisional phase point, i.e.,

$$\mathbf{z} = (\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N, \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_i, \ldots, \boldsymbol{\xi}_j, \ldots \boldsymbol{\xi}_N)$$

with $\mathbf{x}_j = \mathbf{x}_i + \mathbf{n}\sigma$ and $\mathbf{n} \cdot (\boldsymbol{\xi}_i - \boldsymbol{\xi}_j) > 0$,

$$\mathbf{z}' = (\mathbf{x}_1, \ldots, \mathbf{x}_i, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N, \boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_i', \ldots \boldsymbol{\xi}_j', \ldots \boldsymbol{\xi}_N),$$

assumption 2 means that P_0 is continuous outside the contact points and

$$P_0(\mathbf{z}) = P_0(\mathbf{z}'). \tag{2.2.1}$$

In other words, "good" initial probability distributions are those which do not distinguish between precollisional and postcollisional configurations.

There are equations analogous to Eq. (1.2.4) for $P^{(s)}$; they constitute the so-called BBGKY hierarchy:

$$\frac{d}{dt} P^{(s)}(T_\sigma^t \mathbf{z}^s, t) = \left(Q_{s+1}^\sigma P^{(s+1)}\right) \left(T_\sigma^t \mathbf{z}^s, t\right) \tag{2.2.2}$$

(where we have here added an index σ to the flow operators, as a reminder that these operators do change as $\sigma \to 0$). Let us analyse what happens to the collision operator in the Boltzmann–Grad limit.

The operator Q^σ_{s+1}, acting on the time evolved marginal distributions via

$$Q^\sigma_{s+1} P^{(s+1)}(\mathbf{x}_1, \dots \mathbf{x}_s, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_s, t)$$

$$= \sum_{j=1}^{s} (N-s)\sigma^2 \int_{\mathcal{B}} d\mathbf{n} \int d\boldsymbol{\xi}_{s+1} \mathbf{n} \cdot (\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1})\, P^{(s+1)}(\mathbf{x}_1, \dots, \mathbf{x}_s \mathbf{x}_j - \mathbf{n}\sigma, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_{s+1}, t) \tag{2.2.3}$$

is well defined for all t and almost all $\mathbf{z}^s$. Moreover, we can prove

Theorem 2.2.1. *Under the assumptions* 1 *and* 2*,* $Q^\sigma_{s+1} P^{(s+1)}(T^t \mathbf{z}^s, t)$ *is continuous in* t *for almost all* $\mathbf{z}^s$*, and the* $P^s(\cdot, t)$*,* $1 \le s \le N$*, satisfy the* BBGKY *hierarchy in the mild sense, i.e.,*

$$\frac{d}{dt}[P^{(s)}(T^t \mathbf{z}^s, t)] = Q^\sigma_{s+1} P^{(s+1)}(T^t \mathbf{z}^s, t) \tag{2.2.4}$$

for almost all $\mathbf{z}^s$*.*

We now consider the collision operator and split the integration over $\mathcal{B}$ into integrations over two hemispheres: On the hemisphere given by $(\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \cdot \mathbf{n} \le 0$ (incoming configurations), we leave the argument of $P^{(s+1)}$ untouched, but we make here the change $\mathbf{n} \to -\mathbf{n}$ and therefore change this part of the integral to an integral over the hemisphere $(\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \cdot \mathbf{n} \ge 0$.

On the hemisphere given originally by this latter inequality (outgoing configurations), we leave n untouched, but we take advantage of the continuity of $P^{(s+1)}$ through collisions to replace the velocities $\boldsymbol{\xi}_j$ and $\boldsymbol{\xi}_{s+1}$ by their precollisional counterparts $\boldsymbol{\xi}'_j$ and $\boldsymbol{\xi}'_{s+1}$. The result of these operations is

$$\begin{aligned} Q^\sigma_{s+1} P^{(s+1)}(\mathbf{x}_1, \dots, \mathbf{x}_s, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_s) &= \sum_{j=1}^{s} (N-s)\sigma^2 \int d\boldsymbol{\xi}_{s+1} \int_{\mathbf{n}\cdot(\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \ge 0} d\mathbf{n} \\ \mathbf{n} \cdot (\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \Big\{ & P^{(s+1}(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_j - \sigma n, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}'_j, \dots, \boldsymbol{\xi}'_{s+1}) \\ & - P^{(s+1}(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_j + \sigma n, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_j, \dots, \boldsymbol{\xi}_{s+1}) \Big\}. \end{aligned} \tag{2.2.5}$$

In the Boltzmann–Grad limit, $N\sigma^2 \to \alpha$ and formally $Q^\sigma \to Q$, where

$$\begin{aligned} Q_{s+1} f^{(s+1)}(\mathbf{x}_1, \dots, \mathbf{x}_s, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_s) &= \alpha \sum_{j=1}^{s} \int d\boldsymbol{\xi}_{s+1} \int_{\mathbf{n}\cdot(\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \ge 0} d\mathbf{n}\, \mathbf{n} \cdot (\boldsymbol{\xi}_j - \boldsymbol{\xi}_{s+1}) \\ & \Big\{ f^{(s+1)}(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_j, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}'_j, \dots, \boldsymbol{\xi}'_{s+1}) \\ & - f^{(s+1)}(\mathbf{x}_1, \dots, \mathbf{x}_j, \dots, \mathbf{x}_j, \boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_j, \dots, \boldsymbol{\xi}_{s+1}) \Big\}. \end{aligned} \tag{2.2.6}$$

As for fixed s $T^t_\sigma \mathbf{z}^s \to T^t_0 \mathbf{z}^s$ for almost all $\mathbf{z}^s$ in the limit $\sigma \to 0$ (T^t_0 denotes collisionless flow), we expect that the $P^{(s)}$ will converge to a sequence of functions $f^{(s)}$ solving the Boltzmann hierarchy:

$$\frac{d}{dt} f^{(s)}(T^t_0 \mathbf{z}^s, t) = Q_{s+1} f^{(s+1)}(T^t_0 \mathbf{z}^s, t). \tag{2.2.7}$$

The relationship of the Boltzmann hierarchy (2.2.6) to the Boltzmann equation is the following: If $f(\cdot, t)$ solves the Boltzmann equation, then

$$f^{(s)}(\mathbf{x}_1, \ldots \mathbf{x}_s, \boldsymbol{\xi}_1, \ldots \boldsymbol{\xi}_s; t) = \prod_{j=1}^{s} f(\mathbf{x}_j, \boldsymbol{\xi}_j; t)$$

solves the Boltzmann hierarchy. Thus, if the $f^{(s)}$ in (2.2.3) factorize initially and *if* the factorization is preserved in time (the second *if*, usually referred to as propagation of chaos, must be proved), the Boltzmann hierarchy and the Boltzmann equation are equivalent.

By proving the convergence $P^{(s)} \to f^{(s)}$ and propagation of chaos, one completes the objective of validating the Boltzmann equation. First, however, we make some observations which will clarify what we can expect to achieve.

In the derivation of the operator Q, we chose to represent collision phase points in terms of ingoing configurations. Given the assumed continuity along trajectories, we could as well use the representation in terms of outgoing configurations, and that would lead formally to a limit which is equation (2.2.6) with a minus sign in front of the collision operator. Also, if we take the formal limit in the right-hand side of equation (2.2.3) without first splitting into gain and loss terms, we obtain zero, because the integrations over the two hemispheres compensate each other. We are thus compelled to ask whether the representation in terms of ingoing configurations is the right one, i.e., physically meaningful. A more careful analysis of the validity problem shows that the representation in terms of ingoing configurations follows automatically from hard sphere dynamics and is, indeed, not a matter of an a priori choice.

We consider now equation (2.2.3) for $s = 1$ and discuss the propagation of chaos. Assuming representation in terms of ingoing configurations, the right-hand side reads

$$(N-1)\sigma^2 \int_{\Re^3} d\boldsymbol{\xi}_2 \int_{\mathbf{n}\cdot(\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2) \geq 0} d\mathbf{n}\ \mathbf{n} \cdot (\boldsymbol{\xi}_1 - \boldsymbol{\xi}_2)$$

$$\{P^{(2)}(\mathbf{x}_1 + t\boldsymbol{\xi}_1, \mathbf{x}_1 + t\boldsymbol{\xi}_1 - \mathbf{n}\sigma, \boldsymbol{\xi}'_1, \boldsymbol{\xi}'_2; t) - P^{(2)}(\mathbf{x}_1 + t\boldsymbol{\xi}_1, \mathbf{x}_1 + t\boldsymbol{\xi}_1 + \mathbf{n}\sigma, \boldsymbol{\xi}_1, \boldsymbol{\xi}_2; t)\}. \tag{2.2.8}$$

In order to get the right-hand side of the Boltzmann equation we seem to need the crucial assumption that in the limit $N \to \infty$, $\sigma \to 0$ and $N\sigma^2 \to \alpha > 0$ there is a function $f = f(x, \boldsymbol{\xi}, t)$ such that

$$\lim_{N\to\infty} P^{(1)}(\mathbf{x}, \boldsymbol{\xi}, t) = f(\mathbf{x}, \boldsymbol{\xi}, t),$$

$$\lim_{N\to\infty} P^{(2)}(\mathbf{x},\mathbf{x}+\mathbf{n}\sigma,\boldsymbol{\xi}_1,\boldsymbol{\xi}_2;t) = f(\mathbf{x},\boldsymbol{\xi}_1,t)f(\mathbf{x},\boldsymbol{\xi}_2,t) \tag{2.2.9}$$

provided that the configuration is *ingoing*. If this convergence holds, we get the Boltzmann equation in the mild formulation

$$\frac{d}{dt}f(\mathbf{x}+t\boldsymbol{\xi},\boldsymbol{\xi},t) = \alpha\int d\boldsymbol{\xi}_*\int_{\mathcal{B}} d\mathbf{n}\,\mathbf{n}\cdot(\boldsymbol{\xi}-\boldsymbol{\xi}_*)\,(f'f'_*-ff_*)\,(\mathbf{x}+t\boldsymbol{\xi},\boldsymbol{\xi},t).$$

Our convention here is that $f_*(\mathbf{x}+t\boldsymbol{\xi},\boldsymbol{\xi},t) = f(\mathbf{x}+t\boldsymbol{\xi},\boldsymbol{\xi}_*,t)$, etc.

It turns out that (2.2.9) is a statement stronger than what we need. Worse, (2.2.9) can be violated even at time $t=0$ for quite reasonable $P^{(2)}$'s, as can be shown by examples. The form of propagation of chaos which we will be able to prove is that

$$P^{(2)}(\mathbf{x}_1,\mathbf{x}_2,\boldsymbol{\xi}_1,\boldsymbol{\xi}_2;t) \to f(\mathbf{x}_1,\boldsymbol{\xi}_1,t)f(\mathbf{x}_2,\boldsymbol{\xi}_2,t)$$

for almost all $\mathbf{x}_1,\mathbf{x}_2,\boldsymbol{\xi}_1,\boldsymbol{\xi}_2$ (and not on a manifold of codimension one, as in (2.2.9)).

There exists an example[2] of a discrete velocity model for which the derivation done in the present section fails completely.

Given that convergence of the derivatives is not to be expected, what we are going to do is to look at the solution of the BBGKY hierarchy and the Boltzmann hierarchy as a whole (and not at their derivatives) and show that the first converge a.e. to the second. The solution concept which allows us to do this is a series solution concept which we now introduce.

After integration from 0 to t, we get from (2.2.2) that

$$P^{(s)}(T_\sigma^t\mathbf{z}^s,t) = P_0^{(s)}(\mathbf{z}^s) + \int_0^t dt_1\,\left(Q_{s+1}^\sigma P^{(s+1)}\right)\left(T_\sigma^{t_1}\mathbf{z}^s,t_1\right)$$

or

$$P^{(s)}(\mathbf{z}^s,t) = \left(S_\sigma(t)P_0^{(s)}\right)(\mathbf{z}^s) + \int_0^t dt_1\,S_\sigma(t-t_1)Q_{s+1}^\sigma P^{(s+1)}(\mathbf{z}^s,t_1)$$

where $S_\sigma(t)f(\mathbf{z}^s) = f\left(T_\sigma^{-t}\mathbf{z}^s\right)$.

By iterating the last equation $N-s$ times and using the convention that $P_0^{(s)}=0$ for $s>N$, we can express $P^{(s)}(\mathbf{z}^s,t)$ as a finite sum of multiple integrals involving only the functions $P_0^{(r)}$ for $r\geq s$:

$$P^{(s)}(\mathbf{z}^s,t) = \sum_{n=0}^{\infty}\int_0^t dt_1\int_0^{t_1} dt_2,\ldots,$$

$$\int_0^{t_{n-1}} dt_n S_\sigma(t-t_1)Q_{s+1}^\sigma S_\sigma(t_1-t_2),\ldots,Q_{s+n}^\sigma S_\sigma(t_n)P_0^{(s+1)}(\mathbf{z}^s) \tag{2.2.10}$$

Note that the sum is actually finite because of our convention. For $s=N$ (2.2.10) reduces to $P^{(N)}(\mathbf{z},t) = S_\sigma(t)P_0^{(N)}(\mathbf{z})$, which is just the solution of the so-called

Liouville equation, an exact partial differential equation which rules the time evolution of $P^{(N)}(\mathbf{z}, t)$.

Equation (2.2.10) is an equality which holds for almost all $\mathbf{z}^s$. Similarly, a formal series solution can be written down for the Boltzmann hierarchy (2.2.7). It is

$$f^{(s)}(\cdot, t) = \sum_{n=0}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2, \ldots,$$

$$\int_0^{t_{n-1}} dt_n S_0(t - t_1) Q_{s+1} S_0(t_1 - t_2), \ldots, Q_{s+n} S_0(t_n) f_0^{(s+n)} \tag{2.2.11}$$

where

$$S_0(t) f(\mathbf{z}^s) = f(T_0^{-t} \mathbf{z}^s).$$

In contrast to (2.2.10), (2.2.11) is an infinite series, and the question of convergence becomes critical.

There is an obvious trace problem in the definition of Q on L^1-functions; the series solution concept which we adopt nicely avoids this problem, because each term of the series (2.2.11) involves $f_0^{(s)}$ evaluated at phase points which are computed by repeatedly adjoining collision partners (this is what Q does) and backward free streaming (this is what S_0 does), such that each term in the right-hand side of (2.2.11) makes sense if $f_0^{(s)}$ is assumed to be sufficiently smooth.

We emphasize at this point that (2.2.10) and (2.2.11) are profoundly different, in spite of their formal similarity. From a physical point of view, (2.2.10) describes a Hamiltonian (reversible) dynamical system, while (2.2.11) describes a dissipative evolution which is compatible with the H-Theorem. Also, technically speaking, Q is more singular than Q^σ: Indeed, Q_{s+1} involves the trace of $f^{(s+1)}$ on a manifold of codimension 3, while Q_{s+1}^σ needs the trace of $P^{(s+1)}$ on a manifold of codimension 1 (the sphere shrinks to a point in the limit).

On the other hand, the presence of the flow T_σ^t in (2.2.10) makes it hard to interpret the BBGKY hierarchy from a pure PDE point of view. The hierarchy in equation (2.2.2) is a family of equations which can only be established once the flow T_σ^t is defined and once the properties of this flow are well understood.

We are now able to formulate our rigorous validity result. Consider a system of N particles in a region Ω. We shall assume either $\Omega = \Re^3$ or $\Omega \subset \Re^3$ bounded, with a smooth boundary. T_σ^t and T_0^t will refer to the N-particle dynamics and the free flow, both with reflecting boundary conditions on $\partial\Omega$. The case in which Ω is a rectangle with periodic boundary conditions can be considered as well.

Suppose that $f_0^{(s)}(\mathbf{z}^s) = \prod_{i=1}^s f_0(\mathbf{x}_i, \boldsymbol{\xi}_i)$ is the factorizing initial value for the s-th equation in the Boltzmann hierarchy (molecular chaos or statistical independence is taken for granted at $t = 0$), and that $P_0^{(s)}(\mathbf{z}^s)$ is the initial value for the s-th equation in the BBGKY hierarchy. We send $N \to \infty$, $\sigma \to 0$ in such a way that $N\sigma^2 = \alpha$ and assume that

i) if $\left(\Omega \times \Re^3\right)_{\neq}^{s,\sigma} = \left\{\mathbf{z}^s \in \Omega^s \times \Re^3;\ |\mathbf{x}_i - \mathbf{x}_j| > \sigma,\ i \neq j,\ \sigma \geq 0\right\}$, then the $P_0^{(s)}$ are continuous on $\left(\Omega \times \Re^3\right)_{\neq}^{s,\sigma}$ and at the collision points (continuity along trajectories). f_0 is continuous and $\lim_{N\to\infty} P_0^{(s)} = f_0^{(s)}$ uniformly on compact subsets of $\left(\Omega \times \Re^3\right)_{\neq}^{s,\sigma}$ for all $s = 1, 2, \ldots$;

ii) there are positive constants β, C and b such that

$$\sup_{\mathbf{z}^s} P_0^{(s)}(\mathbf{z}^s) \exp\left\{\beta \sum_{i=1}^{s} |\boldsymbol{\xi}_i|^2\right\} \leq C \cdot b^s \tag{2.2.12}$$

for all s.

Finally we can state Lanford's theorem:

Theorem 2.2.2. *Suppose that* i) *and* ii) *hold. Then, on a sufficiently small interval* $[0, t_0]$*, the series solution* $P^{(s)}(\cdot, t)$ *of the* BBGKY *hierarchy converges in the Boltzmann–Grad limit almost everywhere to the series solution of the Boltzmann hierarchy* $f^{(s)}(\cdot, t)$*. This solution exists, is unique and is of the form*

$$f^{(s)}(\mathbf{z}^s, t) = \prod_{i=1}^{s} f(\mathbf{x}_i, \boldsymbol{\xi}_i, t),$$

where f *is a mild solution of the Boltzmann equation to the initial value* f_0*.*

For the proof of this and other results in this section, we refer to a previously quoted monograph[2].

Lanford's method gives a local result for rather general initial values. However, for suitably small initial data one can prove global validity by replacing the smallness condition on time by a largeness condition on the mean free path; consider, for example, hard sphere dynamics in all of $\Re^3$ and initial data which decay sufficiently fast at infinity, a situation which we address in this section.

First, we note that certain steps of the proof discussed in the previous section are completely general; therefore, a global result will be proved if we can control the series solution for the BBGKY and Boltzmann hierarchies globally.

As before, we assume a factorizing initial value

$$f_0^{(s)}(\mathbf{z}^s) = \prod_{i=1}^{s} f_0(\mathbf{x}_i, \boldsymbol{\xi}_i)$$

and the Boltzmann–Grad limit $N \to \infty$, $\sigma \to 0$, $N\sigma^2 = \alpha$.

In addition, suppose that

i) the $P_\sigma^{(s)}(\cdot, 0)$ are continuous on $(\Re^3 \times \Re^3)_{\neq}^{s,\sigma}$ and

$$\lim_{N\to\infty} P_\sigma^{(s)}(\cdot, 0) = f_0^{(s)}$$

uniformly on compact subsets of $(\Re^3 \times \Re^3)_{\neq}^{s,0}$.

ii) there are constants $\beta_0 > 0$, $c > 0$ and $b > 0$ such that

$$\sup_{\mathbf{z}^s} \left(P_\sigma^{(s)}(\mathbf{z}^s, 0) \exp\left(\beta_0 \sum_{i=1}^{s} (|\boldsymbol{\xi}_i|^2 + |\mathbf{x}_i|^2) \right) \right) \leq cb^s.$$

Under these hypotheses, we have[4,5]

Theorem 2.2.3. *Suppose that* i) *and* ii) *hold. Then, if $b\alpha$ is sufficiently small, the series solution $P_\sigma(\cdot, t)$ of the* BBGKY *hierarchy converges for all $t > 0$ in the Boltzmann–Grad limit almost everywhere to the series solution $f(\cdot, t)$ of the Boltzmann hierarchy. The latter factorizes as*

$$f^{(s)}(\mathbf{z}^s, t) = \prod_{i=1}^{s} f(\mathbf{x}_i, \boldsymbol{\xi}_i, t)$$

and f is a mild global solution of the Boltzmann equation for the initial value f_0. Moreover, $P_\sigma^{(s)}$ and $f^{(s)}$ satisfy the estimates

$$0 \leq P_\sigma^{(s)}(\mathbf{z}^s, t) \leq (cb)^s \exp(-\beta_0 \cdot I(T^{-t}\mathbf{z}^s))$$

(where $I(\mathbf{z}^s) = \sum_{i=1}^{s} \mathbf{x}_i^2$),

$$0 \leq f(\mathbf{x}, \boldsymbol{\xi}, t) \leq (c \cdot b) \exp\left(-\beta_0 (\mathbf{x} - t\boldsymbol{\xi})^2\right).$$

The constant c is independent of N and s.

For the proof we refer again to the previously quoted monograph[2].

2.3 Existence and Uniqueness Results

The well-posedness of the initial value problem (IVP in the sequel) for the Boltzmann equation means that we prove that there is a unique nonnegative solution preserving the energy and satisfying the H-Theorem, from a positive initial datum with finite energy and entropy. However, for general initial data, it is difficult, and until now not known, whether such a well-behaved solution can be constructed globally in time. The difficulty in doing this is obviously related to the nonlinearity of the collision operator and the apparent lack of conservation laws or a priori estimates preventing the solution from becoming singular in finite time.

A complete validity discussion for the Boltzmann equation will automatically contain existence and uniqueness results. Consequently, by the discussion of the previous section, we already have some existence and uniqueness theorems. Unfortunately, a validity proof involves several hard additional steps beyond existence and uniqueness, like estimates for the BBGKY hierarchy. Therefore, the Boltzmann equation has been validated rigorously only in the few simple situations which we discussed in the previous section (locally in time, and globally for a rare gas cloud in all space).

Existence (and in some situations uniqueness) of solutions to IVP is known for a much larger variety of cases, and it is our purpose now to survey these results.

When the distribution function of a gas is not depending on the space variable, the equation is considerably simplified. The collision operator is basically Lipschitz continuous in L^1_+ and the equation becomes globally solvable in time. Moreover, uniqueness, asymptotic behavior and a theory of classical solutions have been established. The theory for the spatially homogeneous Boltzmann equation begins in the early 1930s and can be considered rather complete; unfortunately the homogeneous case is hardly of interest for applications. The reader interested in this theory should consult the previously cited monograph[2].

If the solution is initially sufficiently close to a Maxwellian, it is possible to prove that a solution can be constructed globally in time, and we have uniqueness and asymptotic behavior. The approach is based on the analysis of the linearized Boltzmann operator, which leads us to a differential inequality of the type

$$\frac{d}{dt}y \leq -ky + y^2$$

where $y = y(t)$ is some norm of the deviation of the solution from the Maxwellian and k is a positive number. Therefore, if $y(0)$ is sufficiently small, we can control the solution for all times. As we said, the basic ingredient is good control of the linearized Boltzmann operator. This theory will be discussed in the next chapter.

The case of perturbation of a vacuum has already been discussed in the previous section, together with the local existence theory.

If the initial value is close to a homogeneous distribution, a solution starting from it can be constructed globally in time. Uniqueness and asymptotic behavior can also be proved. The main idea is explained in Chapter VII, Section 5 of Cercignani et al[2].

Except the first one, all these results have a perturbation character. The knowledge of particular solutions helps to construct other solutions which are close to the original ones. The general IVP is poorly understood, although a significant and somewhat unexpected step was performed in the late 1980s. Consider an equation similar to the Boltzmann equation for which we have conservation of mass and energy and the H-Theorem. Denote by $f^\epsilon(t)$ the solutions. Here, ϵ is a regularization parameter such that the solutions formally converge to a solution of the Boltzmann equation in the limit $\epsilon \to 0$. The conservation laws yield the existence of a weak limit denoted by $f(t)$. However, since the collision operator is quadratic in f, it cannot be weakly continuous. Thus it does not follow by general arguments that $f(t)$ solves the Boltzmann equation. Nevertheless, some smoothness gained by the streaming operator gives enough compactness to prove that $f(t)$ actually solves the Boltzmann equation in the mild sense.

The method gives neither uniqueness nor energy conservation, but the entropy is seen to decrease along the solution trajectories.

Let us begin with some notation and a rather standard definition. Let Λf denote the left-hand side of the Boltzmann equation and

$$f^{\#}(\mathbf{x}, \boldsymbol{\xi}, t) = f(\mathbf{x} + \boldsymbol{\xi} t, \, \boldsymbol{\xi}, t).$$

Definition 2.3.1. A measurable function $f = f(\mathbf{x}, \boldsymbol{\xi}, t)$ on $[0, \infty) \times \Re^3 \times \Re^3$ is a mild solution of the Boltzmann equation for the (measurable) initial value $f_0(\mathbf{x}, \boldsymbol{\xi})$ if for almost all $(\mathbf{x}, \boldsymbol{\xi})$ $Q_\pm(f, f)^{\#}(\mathbf{x}, \, \boldsymbol{\xi}, \, \cdot)$ are in $L^1_{\text{loc}}[0, \infty)$, and if for each $t \geq 0$,

$$f^{\#}(\mathbf{x}, \boldsymbol{\xi}, t) = f_0(\mathbf{x}, \boldsymbol{\xi}) + \int_0^t Q(f, f)^{\#}(\mathbf{x}, \, \boldsymbol{\xi}, \, s) \, ds.$$

One of the key ideas used by DiPerna and Lions to prove a general existence theorem was to relax the solution concept even further, such that the bounds provided by the energy conservation and the H-theorem could be put to the best use, and then to regain mild solutions via a limit procedure. They called the relaxed solution concept "renormalized solution" and defined it in the following way:

Definition 2.3.2. A function $f = f(\mathbf{x}, \boldsymbol{\xi}, t) \in L^1_+(\Re^+_{\text{loc}} \times \Re^3 \times \Re^3)$ is called a renormalized solution of the Boltzmann equation if

$$\frac{Q_\pm(f, f)}{1 + f} \in L^1_{\text{loc}}(\Re_+ \times \Re^3 \times \Re^3 \tag{2.3.1}$$

and if for every Lipschitz continuous function $\beta : \Re_+ \to \Re$ which satisfies $|\beta'(t)| \leq C/(1 + t)$ for all $t \geq 0$ one has

$$\Lambda\beta(f) = \beta'(f) Q(f, f) \tag{2.3.2}$$

in the sense of distributions.

DiPerna and Lions[3] noticed that renormalization would actually give mild solutions, according to the following.

Lemma 2.3.1. *Let $f \in (L^1_{\text{loc}} \times \Re^3 \times \Re^3)$. If f satisfies* (2.3.1) *and* (2.3.2) *with $\beta(t) = \ln(1+t)$, then f is a mild solution of the Boltzmann equation. If f is a mild solution of the Boltzmann equation and if $Q_\pm(f, f)/(1 + f) \in L^1_{\text{loc}}(\Re_+ \times \Re^3 \times \Re^3)$, then f is a renormalized solution.*

Their main result is:

Theorem 2.3.2. (DiPerna and Lions[3]) *Suppose that $f_0 \in L^1_+(\Re^3 \times \Re^3$ is such that*

$$\int_{\Re^3} \int_{\Re^3} f_0 (1 + |\mathbf{x}|^2 + |\boldsymbol{\xi}|^2) \, d\mathbf{x} \, d\boldsymbol{\xi} < \infty$$

and

$$\int_{\Re^3} \int_{\Re^3} f_0 |\ln f_0| \, d\mathbf{x} \, d\boldsymbol{\xi} < \infty.$$

Then there is a renormalized solution of the Boltzmann equation such that $f \in C(\Re_+, L^1(\Re^3, \Re^3), \, f \big|_{t=0} = f^0$.

2.4 Remarks on the Mathematical Theory of the Boltzmann Equation

The existence theorem of DiPerna and Lions is rightly considered as a basic result of the mathematical theory of the Boltzmann equation. Unfortunately, it is far from providing a complete theory, since there is no proof of uniqueness; in addition, there is no proof that energy is conserved and conservation of momentum can be proved only globally and not locally. More complete results concerning conservation equations are only known in the case of solutions depending on just one space coordinate[1].

Fortunately, a more complete theory is available for slow flows, to which the present book is devoted. In this case, one can exploit the fact that the distribution function is close to a space homogeneous Maxwellian to take advantage of rigorous perturbation methods, as we shall do in the next chapter.

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Chapter 3

Perturbations of Equilibria

3.1 The Linearized Collision Operator

Our first aim in this chapter will be to find a global solution $f = f(\mathbf{x}, \boldsymbol{\xi}, t)$ of the Cauchy problem for the Boltzmann equation for hard spheres:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f) \tag{3.1.1}$$

when f is close to some absolute Maxwellian M, which without loss of generality (thanks to possible scalings and choice of a suitable reference frame) can be assumed to be $(2\pi)^{-3/2} \exp(-|\boldsymbol{\xi}|^2/2)$. To this end we introduce a new unknown h related to the distribution function f by

$$f = M + M^{1/2} h. \tag{3.1.2}$$

The Boltzmann equation (3.1.1) takes on the form

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial h}{\partial \mathbf{x}} = Lh + \Gamma(h, h) \tag{3.1.3}$$

where L is the linearized collision operator, defined by

$$Lh = 2M^{-1/2} Q(M^{1/2} h, M) \tag{3.1.4}$$

(here Q is the bilinear operator defined in Eq. (1.4.1) and $\Gamma(h, h)$ is the nonlinear part, which should be small compared to the linear one, and is given by

$$\Gamma(g, h) = M^{-1/2} Q(M^{1/2} g, M^{1/2} h) \tag{3.1.5}$$

with $g = h$.

A more explicit expression of Lh reads as follows:

$$Lh = \int_{\Re^3} \int_{S_+^2} (h' R'_* + R' h'_* - R h_* - h R_*) R_* |\mathbf{V} \cdot \mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n} \tag{3.1.6}$$

where, for convenience, R denotes $M^{1/2}$ and we took into account that $M'M'_* = MM_*$. Because of Eq. (1.4.8) (with Rh in place of f, M in place of g and g/R in place of ϕ), we have the identity

$$\int_{\Re^3} gLhd\boldsymbol{\xi} = -\frac{1}{4}\int_{\Re^3}\int_{\Re^3}\int_{S^2_-}(h'R'_* + R'h'_* - hR_* - Rh_*)$$
$$\times(g'R'_* + R'g'_* - gR_* - Rg_*)|\mathbf{V}\cdot\mathbf{n}|d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\mathbf{n}. \tag{3.1.7}$$

This relation expresses a basic property of the linearized collision term. In order to make it clear, let us introduce the Hilbert space of square summable functions of $\boldsymbol{\xi}$ endowed with the scalar product

$$(g,h) = \int_{\Re^3} \overline{g} h d\boldsymbol{\xi} \tag{3.1.8}$$

where the bar denotes complex conjugation. Then Eq. (3.1.7) (with $\overline{g}$ in place of g) gives (thanks to the symmetry of the expression in the right-hand side of (3.1.7) with respect to the interchange $g \Leftrightarrow h$):

$$(g, Lh) = (Lg, h). \tag{3.1.9}$$

Further,

$$(h, Lh) \leq 0 \tag{3.1.10}$$

and the equality sign holds if and only if

$$h'/R' + h'_*/R'_* - h/R - h_*/R_* = 0, \tag{3.1.11}$$

i.e., unless h/R is a collision invariant.

Eqs. (3.1.9) and (3.1.10) indicate that the operator L (provided it is taken with its maximal domain in L^2) is self-adjoint and nonpositive in L^2. In order to exploit these and other good properties of L, we shall introduce the operator

$$B = L - \boldsymbol{\xi}\cdot\frac{\partial}{\partial\mathbf{x}} \tag{3.1.12}$$

and write Eq. (3.1.3) in the integral form

$$h(t) = T(t)h(0) + \int_0^t dsT(t-s)\Gamma(h(s), h(s)) \tag{3.1.13}$$

where $T(t)$ is the semigroup generated by B. We can hope that in some norm (see Lemma 3.2.6 below)

$$\| \Gamma(h,h) \| \leq C \| h \|^2 ; \tag{3.1.14}$$

then if we could prove (and this would be the crucial estimate) that, for some positive c,

$$\| T(t) \| \leq Ce^{-ct}, \tag{3.1.15}$$

we would have

$$\parallel h(t) \parallel \leq Ce^{-ct} \parallel h(0) \parallel + \int_0^t ds\ e^{-c(t-s)} \parallel h(s) \parallel^2 . \tag{3.1.16}$$

If we let

$$\hat{h} = \sup_t \parallel h(t)e^{ct} \parallel \tag{3.1.17}$$

Eq. (3.1.16) gives

$$\hat{h} \leq C \parallel h(0) \parallel + C\hat{h}^2 \tag{3.1.18}$$

which implies that $\hat{h}$ is bounded whenever $\parallel h(0) \parallel$ is small.

Unfortunately this strategy cannot be followed so easily. In fact, since the dissipative part of B is contained in L, one would like to prove Eq. (3.1.15) for the semigroup generated by L itself. L, however, has five linearly independent eigenfunctions corresponding to the zero eigenvalue; these are the functions h such that h/R is a collision invariant, because then Eq. (3.1.11) holds and, according to Eq. (3.1.6), Lh vanishes. Then $T(t)h = h$ for any linear combination of these eigenfunctions and the desired property does not hold for the semigroup generated by L. The operator $\boldsymbol{\xi} \cdot \partial/\partial\mathbf{x}$, however, generates a semigroup, which, although norm-preserving, has the tendency to spread the molecular distribution in a uniform way; this will help in obtaining the desired estimate in $\Re^3$. In fact to prove this estimate will be our major aim in the following sections. This will require a preliminary study of the spectral properties of L and of the Fourier transform of $B, B(\mathbf{k})$.

3.2 The Basic Properties of the Linearized Collision Operator

In order to study the linearized collision operator L, given by Eq. (3.1.6), we start by remarking that we can split L as $K - \nu(|\boldsymbol{\xi}|)I$, where $K = K_2 - K_1$ is an integral operator, I the identity and ν a function bounded from below by a constant ν_0 and from above by a linear function. Specifically

$$\nu(|\boldsymbol{\xi}|) = \int_{\Re^3} \int_{S_+^2} M_* |\mathbf{V} \cdot \mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n},$$

$$K_1 h = R(|\boldsymbol{\xi}|) \int_{\Re^3} \int_{S_+^2} h_* R_* |\mathbf{V} \cdot \mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n}, \tag{3.2.1}$$

$$K_2 h = \int_{\Re^3} \int_{S_+^2} (h' R'_* + R' f'_*) R_* |\mathbf{V} \cdot \mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n}.$$

It is easy to pick out the kernel of K_1, $k_1(\boldsymbol{\xi}, \boldsymbol{\xi}_*)$ by inspection:

$$k_1(\boldsymbol{\xi}, \boldsymbol{\xi}_*) = \pi |\boldsymbol{\xi} - \boldsymbol{\xi}_*| R(|\boldsymbol{\xi}|) R(|\boldsymbol{\xi}_*|). \tag{3.2.2}$$

To find the kernel of K_2 requires a little more work. To reduce it a little bit we make use of a trick. Let us consider a unit vector $\mathbf{m}$ that lies in the plane of $\mathbf{V}$ and $\mathbf{n}$ and is orthogonal to $\mathbf{n}$. We can then write $\mathbf{V} = \mathbf{n}(\mathbf{n}\cdot\mathbf{V})+\mathbf{m}(\mathbf{m}\cdot\mathbf{V})$, which implies $\boldsymbol{\xi}-\mathbf{n}(\mathbf{n}\cdot\mathbf{V}) = \boldsymbol{\xi}_*+\mathbf{m}(\mathbf{m}\cdot\mathbf{V})$, $\boldsymbol{\xi}_*+\mathbf{n}(\mathbf{n}\cdot\mathbf{V}) = \boldsymbol{\xi}-\mathbf{m}(\mathbf{m}\cdot\mathbf{V})$; thus if we use $\mathbf{m}$ in place of $\mathbf{n}$ in the second part of the integral appearing in (3.2.1), it becomes identical to the first, except for the fact that θ is replaced by $\pi/2-\theta$ (and ϕ by $\phi\pm\pi$). But even this difference disappears, because $|\mathbf{V}\cdot\mathbf{n}|d\mathbf{n} = |\mathbf{V}|\cos\theta\sin\theta d\theta d\phi = |\mathbf{V}\cdot\mathbf{m}|d\mathbf{m}$. Thus

$$K_2 h = 2\int_{\Re^3}\int_{S^2_+} h' R'_* R_* |\mathbf{V}\cdot\mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n} = \int_{\Re^3}\int_{S^2} h' R'_* R_* |\mathbf{V}_*\cdot\mathbf{n}| d\mathbf{V}_* d\mathbf{n} \tag{3.2.3}$$

where in the last integral $\mathbf{n}$ runs over the entire sphere S^2 and $\mathbf{V}_* = \boldsymbol{\xi}_* - \boldsymbol{\xi}$ is used as an integration variable in place of $\boldsymbol{\xi}_*$ (a unit Jacobian transformation). Next consider the components of $\mathbf{V}_*$ parallel and perpendicular to $\mathbf{n}$:

$$\mathbf{V}_* = \mathbf{v}+\mathbf{w};\qquad \mathbf{v} = \mathbf{n}(\mathbf{n}\cdot\mathbf{V}_*);\qquad \mathbf{w} = \mathbf{V}_* - \mathbf{n}(\mathbf{n}\cdot\mathbf{V}_*). \tag{3.2.4}$$

We now perform the integration in Eq. (3.2.3) in the following order: first we integrate with respect to $\mathbf{w}$ (on a plane Π perpendicular to $\mathbf{n}$), then w.r.t. $\mathbf{v}$, then w.r.t. $\mathbf{n}$. With $\mathbf{n}$ fixed, the replacement of $\mathbf{V}_*$ by $\mathbf{v}$ and $\mathbf{w}$ is just a choice of coordinates. After integrating with respect to $\mathbf{w}$, we combine the one-dimensional $\mathbf{v}$-integration in the direction $\mathbf{n}$ with the integral with respect to $\mathbf{n}$ over the unit sphere to give a three-dimensional integration over the vector $\mathbf{v} = |\mathbf{v}|\mathbf{n}$; here we must introduce a factor 2 because $\mathbf{v}$ describes $\Re^3$ twice (for a given $\mathbf{V}_*$, $\mathbf{n}$ and $-\mathbf{n}$ give the same point). Thus since the Jacobian from $d\mathbf{v}$ to $d\mathbf{n}d|\mathbf{v}|$ is $|\mathbf{v}|^2$, we have

$$d\mathbf{n}d\mathbf{V}_* = 2|\mathbf{v}|^{-2} d\mathbf{v}d\mathbf{w}, \tag{3.2.5}$$

and Eq. (3.2.3) becomes

$$K_2 h = 2\int_{\Re^3}\int_{\Pi} h(\boldsymbol{\xi}+\mathbf{v})R(\boldsymbol{\xi}+\mathbf{v}+\mathbf{w})R(\boldsymbol{\xi}+\mathbf{w})|\mathbf{v}|^{-1} d\mathbf{w}d\mathbf{v} \tag{3.2.6}$$

where the integration with respect to $\mathbf{w}$ over Π (the plane through the origin perpendicular to $\mathbf{v}$) has to be performed first. The kernel of the integral operator K_2 is now clear: introducing the new variable $\boldsymbol{\xi}_* = \mathbf{v}+\boldsymbol{\xi}$, the kernel is

$$k_2(\boldsymbol{\xi},\boldsymbol{\omega}) = 2|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1}\int_{\Pi} R(\boldsymbol{\xi}_*+\mathbf{w})R(\boldsymbol{\xi}+\mathbf{w})d\mathbf{w} \tag{3.2.7}$$

where Π is now perpendicular to $\boldsymbol{\xi}-\boldsymbol{\xi}_*$. Since

$$|\boldsymbol{\xi}_*+\mathbf{w}|^2+|\boldsymbol{\xi}+\mathbf{w}|^2 = \boldsymbol{\xi}_*^2+\boldsymbol{\xi}^2+2(\boldsymbol{\xi}_*+\boldsymbol{\xi})\cdot\mathbf{w}+2|\mathbf{w}|^2 = 2|\mathbf{w}+\frac{1}{2}(\boldsymbol{\xi}_*+\boldsymbol{\xi})|^2+\frac{1}{2}|\boldsymbol{\xi}_*-\boldsymbol{\xi}|^2, \tag{3.2.8}$$

$$R(\boldsymbol{\xi}_*+\mathbf{w})R(\boldsymbol{\xi}+\mathbf{w}) = R(2^{1/2}\mathbf{w}+2^{-1/2}(\boldsymbol{\xi}_*+\boldsymbol{\xi}))R(2^{-1/2}(\boldsymbol{\xi}_*-\boldsymbol{\xi})). \tag{3.2.9}$$

The vector $\frac{1}{2}(\boldsymbol{\xi}_* + \boldsymbol{\xi})$ has a part in the plane Π, say $\mathbf{u}$, which can be eliminated by letting $\mathbf{z} = \mathbf{w} + \mathbf{u}$ (a translation in Π); the remaining part is the projection on the direction of $\boldsymbol{\xi}_* - \boldsymbol{\xi}$, i.e.,

$$\frac{1}{2}(\boldsymbol{\xi}_* + \boldsymbol{\xi}) \cdot \frac{\boldsymbol{\xi}_* - \boldsymbol{\xi}}{|\boldsymbol{\xi}_* - \boldsymbol{\xi}|} = \frac{1}{2} \frac{|\boldsymbol{\xi}_*|^2 - |\boldsymbol{\xi}|^2}{|\boldsymbol{\xi}_* - \boldsymbol{\xi}|}. \tag{3.2.10}$$

By means of Eqs. (3.2.9) and (3.2.10), Eq. (3.2.7) becomes

$$\begin{aligned} k_2(\boldsymbol{\xi}, \boldsymbol{\xi}_*) = 2(2\pi)^{3/4}|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1} R(2^{-1/2}\frac{|\boldsymbol{\xi}_*|^2 - |\boldsymbol{\xi}|^2}{|\boldsymbol{\xi}_* - \boldsymbol{\xi}|}) \\ \times R(2^{-1/2}(\boldsymbol{\xi}_* - \boldsymbol{\xi})) \int_{\Pi} R(2^{1/2}\mathbf{z}) d\mathbf{z}. \end{aligned} \tag{3.2.11}$$

The integral is now easily performed with the result $(2\pi)^{-3/4}2\pi = (2\pi)^{-1/4}$ and Eq. (3.2.11) becomes

$$k_2(\boldsymbol{\xi}, \boldsymbol{\xi}_*) = 4\pi|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1} R(2^{-1/2}\frac{|\boldsymbol{\xi}_*|^2 - |\boldsymbol{\xi}|^2}{|\boldsymbol{\xi}_* - \boldsymbol{\xi}|}) R(2^{-1/2}(\boldsymbol{\xi}_* - \boldsymbol{\xi})). \tag{3.2.12}$$

Finally, we can make the expression for the collision frequency more explicit:

$$\begin{aligned} &\nu(|\boldsymbol{\xi}|) = \int_{\Re^3} \int_{S^2} M_* |\mathbf{V} \cdot \mathbf{n}| d\boldsymbol{\xi}_* d\mathbf{n} \\ &= \pi \int_{\Re^3} M(\boldsymbol{\xi}_*)|\boldsymbol{\xi}_* - \boldsymbol{\xi}| d\boldsymbol{\xi}_* = \int_{\Re^3} M(\boldsymbol{\xi} + \mathbf{v})|\mathbf{v}| d\mathbf{v} \\ &= (2\pi)^{-1/2} \int_0^\infty \int_0^\pi \exp(-|\boldsymbol{\xi}|^2/2 - |\mathbf{v}|^2/2 - |\boldsymbol{\xi}||\mathbf{v}|\cos\theta)|\mathbf{v}|^3 \sin\theta d|\mathbf{v}| d\theta \\ &= (2\pi)^{-1/2}|\boldsymbol{\xi}|^{-1}[\int_0^\infty \exp(-|\boldsymbol{\xi}|^2/2 - t^2/2 + |\boldsymbol{\xi}|t)t^2 dt \\ &\quad - \int_0^\infty \exp(-|\boldsymbol{\xi}|^2/2 - t^2/2 - |\boldsymbol{\xi}|t)t^2 dt] \\ &= (2\pi)^{-1/2}|\boldsymbol{\xi}|^{-1}[\int_{-|\boldsymbol{\xi}|}^\infty \exp(-u^2/2)(u + |\boldsymbol{\xi}|)^2 du - \int_{|\boldsymbol{\xi}|}^\infty \exp(-u^2/2)(u - |\boldsymbol{\xi}|)^2 du] \\ &= (2\pi)^{-1/2}|\boldsymbol{\xi}|^{-1}[2\int_0^{|\boldsymbol{\xi}|} \exp(-u^2/2)(u^2 + |\boldsymbol{\xi}|^2) du + 4|\boldsymbol{\xi}|\exp(-|\boldsymbol{\xi}|^2/2)] \\ &= (2\pi)^{-1/2}[2(|\boldsymbol{\xi}| + |\boldsymbol{\xi}|^{-1}) \int_0^{|\boldsymbol{\xi}|} \exp(-u^2/2) du + 2\exp(-|\boldsymbol{\xi}|^2/2)] \end{aligned} \tag{3.2.13}$$

where we first performed the trivial integration with respect to $\mathbf{n}$, then changed the integration variable from $\boldsymbol{\xi}_*$ to $\mathbf{v} = \boldsymbol{\xi}_* - \boldsymbol{\xi}$ and transformed the resulting integral from Cartesian to polar coordinates in velocity space; then we performed the integration with respect to the angle variables and changed the name of the remaining integration variable from $|\mathbf{v}|$ to t for convenience; the resulting two integrals in t are first transformed by letting $t = u+|\boldsymbol{\xi}|$ and $t = u-|\boldsymbol{\xi}|$ respectively and then, after expanding the squares and simplifying, the last step has been performed by a partial integration.

Thus we have proved the following

Theorem 3.2.1. *The linearized collision operator (defined on the functions $h(.)$ of L^2 such that $[\nu(|.|)]^{1/2}h(.)$ is also in L^2) is self-adjoint and nonpositive in L^2, with a five-fold null eigenspace spanned by $M^{1/2}\psi_\alpha$, where ψ_α $(\alpha = 0, 1, 2, 3, 4)$ are the collision invariants. It can be decomposed into the difference*

$$L = K - \nu(|\boldsymbol{\xi}|)I \tag{3.2.14}$$

where $\nu(|\boldsymbol{\xi}|)$is given by (3.2.13) *and satisfies the bound*

$$0 < \nu_0 \leq \nu(|\boldsymbol{\xi}|) \leq \nu_1(1 + |\boldsymbol{\xi}|^2)^{1/2} \tag{3.2.15}$$

with ν_0 and ν_1 positive numbers, while I is the identity operator and K is an integral operator with a real, measurable, symmetric kernel $k(\boldsymbol{\xi}, \boldsymbol{\xi}_*)$ given by

$$k(\boldsymbol{\xi}, \boldsymbol{\xi}_*) = (2\pi)^{-1/2}2|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1} \exp(-\frac{1}{8}\frac{(|\boldsymbol{\xi}_*|^2 - |\boldsymbol{\xi}|^2)^2}{|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^2} - \frac{1}{8}|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^2)$$

$$-\frac{1}{2}|\boldsymbol{\xi} - \boldsymbol{\xi}_*| \exp[-(|\boldsymbol{\xi}|^2 + |\boldsymbol{\xi}_*|^2)/4]. \tag{3.2.16}$$

For later purposes we shall need estimates of this kernel. It is trivial to prove that

$$k(\boldsymbol{\xi}, \boldsymbol{\xi}_*) \leq (c_1|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1} + c_2|\boldsymbol{\xi} - \boldsymbol{\xi}_*|) \exp(-\frac{1}{8}|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^2). \tag{3.2.17}$$

This estimate has the following consequence:

Theorem 3.2.2. *The kernel of the operator K is integrable and square integrable with respect to $\boldsymbol{\xi}_*$. The integrals are bounded by a constant, independent of $\boldsymbol{\xi}$.*

Proof. The proof is trivial, thanks to (3.2.17), because of the exponential decay of the kernel and the fact that $|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-1}$ and $|\boldsymbol{\xi}_* - \boldsymbol{\xi}|^{-2}$ are integrable in a neighborhood of $\Re^3$ about $\boldsymbol{\xi}$. The fact that the bounds are independent of $\boldsymbol{\xi}$ follows from the fact that the r.h.s. of Eq. (3.2.17) is translation invariant. $\square$

We now prove

Theorem 3.2.3. *The kernel $k(\boldsymbol{\xi}, \boldsymbol{\xi}_*)$ of the operator K is such that for any $r \geq 0$ we have*

$$\int k(\boldsymbol{\xi}, \boldsymbol{\xi}_*)(1 + |\boldsymbol{\xi}_*|^2)^{-r} d\boldsymbol{\xi}_* \leq k_0(1 + |\boldsymbol{\xi}|^2)^{-r-1/2}. \tag{3.2.18}$$

Proof. If we had just $-r$ as an exponent in the right-hand side it would be enough to use estimate (3.2.17). To gain the additional $-1/2$ requires a longer proof . If we look at the explicit expression (3.2.16) we realize that the part after the minus sign (arising from k_2) is easy to deal with, because of the exponential $\exp(-|\boldsymbol{\xi}|^2/4)$. We thus have only to prove that

$$I = (1+|\boldsymbol{\xi}|^2)^{r+1/2}\int(1+|\boldsymbol{\xi}+\mathbf{v}|^2)^{-r}|\mathbf{v}|^{-1}\exp\Big(-\frac{1}{8}\frac{(2\boldsymbol{\xi}\cdot\mathbf{v}+|\mathbf{v}|^2)^2}{|\mathbf{v}|^2}-\frac{1}{8}|\mathbf{v}|^2\Big)d\mathbf{v} \tag{3.2.19}$$

is bounded uniformly in $\boldsymbol{\xi}$. We split the integration into I_1+I_2, where the former refers to $|\mathbf{v}|>|\boldsymbol{\xi}|/4$ and the latter to $|\mathbf{v}|<|\boldsymbol{\xi}|/4$. We have

$$I_1 < (1+|\boldsymbol{\xi}|^2)^{r+1/2}\int_{|\mathbf{v}|>|\boldsymbol{\xi}|/4}|\mathbf{v}|^{-1}\exp\Big(-\frac{1}{8}|\mathbf{v}|^2\Big)d\mathbf{v} \tag{3.2.20}$$

which is obviously bounded. For I_2 we can restrict ourselves to $|\boldsymbol{\xi}|\geq 1$, because otherwise the result is clear. For $|\boldsymbol{\xi}|\geq 1$ we use $1+|\boldsymbol{\xi}+\mathbf{v}|^2>1+9|\boldsymbol{\xi}|^2/16$ and polar coordinates to obtain:

$$\begin{aligned} I_2 &= (1+|\boldsymbol{\xi}|^2)^{r+1/2}(1+9|\boldsymbol{\xi}|^2/16)^{-r} \\ &\quad\times 2\pi\int_0^\infty\int_0^\pi \exp\Big(-\frac{1}{8}(2|\boldsymbol{\xi}|\cos\theta+|\mathbf{v}|)^2-\frac{1}{8}|\mathbf{v}|^2\Big)|\mathbf{v}|\sin\theta d|\mathbf{v}|d\theta \\ &< (1+|\boldsymbol{\xi}|^2)^{r+1/2}(1+9|\boldsymbol{\xi}|^2/16)^{-r}(2\pi)^{1/2}|\boldsymbol{\xi}|^{-1}\int_0^\infty \exp\Big(-\frac{1}{8}|\mathbf{v}|^2\Big)|\mathbf{v}|d|\mathbf{v}| \\ &= 4(1+|\boldsymbol{\xi}|^2)^{r+1/2}(1+9|\boldsymbol{\xi}|^2/16)^{-r}(2\pi)^{1/2}|\boldsymbol{\xi}|^{-1} \end{aligned} \tag{3.2.21}$$

which for $|\boldsymbol{\xi}|\geq 1$ is clearly bounded. In an intermediate step here we have used the inequality

$$\begin{aligned} &\int_0^\pi \exp\Big(-\frac{1}{8}(2|\boldsymbol{\xi}|\cos\theta+|\mathbf{v}|)^2\sin\theta d\theta \\ &< \int_{-\infty}^\infty \exp\Big(-\frac{1}{2}|\boldsymbol{\xi}|^2t^2\Big)dt = (2\pi)^{1/2}|\boldsymbol{\xi}|^{-1}. \end{aligned} \tag{3.2.22}$$

Inequality (3.2.13) is thus proved. □

In the following we shall denote by $B(\mathcal{X},\mathcal{Y})$ the set of all linear bounded operators from a Banach space $\mathcal{X}$ into a Banach space $\mathcal{Y}$, and by $C(\mathcal{X},\mathcal{Y})$ its subset consisting of compact operators. When $\mathcal{Y}=\mathcal{X}$, we simply write $B(\mathcal{X})$ and $C(\mathcal{X})$. We also denote by L^∞_β the Banach space of the functions h such that $(1+|\boldsymbol{\xi}|^2)^{\beta/2}h$ is in $L^\infty(\Re^3)$. Then we can prove

Theorem 3.2.4. *The integral operator K is in $B(L^2) \cap B(L^\infty_\beta, L^\infty_{\beta+1})$, $\beta \geq 0$. It is also in $B(L^2, L^\infty_0)$ and in $C(L^2)$.*

Proof. The fact that $K \in B(L^2, L^\infty_0)$ follows from Theorem 3.2.2. We now prove that $K \in C(L^2)$. Let χ_R the characteristic function of $\{\boldsymbol{\xi} : |\boldsymbol{\xi}| \leq R\}$. Then in $B(L^2)$ we have (thanks to Theorem 2.2.3):

$$\| (1 - \chi_R)K \| < C(1 + R)^{-1} \to 0,$$

$$\| K(1 - \chi_R) \| < C(1 + R)^{-1} \to 0 \qquad (R \to \infty). \tag{3.2.23}$$

In order to prove these results we apply the Schwarz inequality in a suitable way; we just indicate how to prove the first of these relations:

$$\begin{aligned}
&\| (1 - \chi_R)K \|^2 = \sup_{\|h\|=1} \int d\boldsymbol{\xi} (1 - \chi_R(\boldsymbol{\xi})) \left[\int d\boldsymbol{\omega} k(\boldsymbol{\xi}, \boldsymbol{\omega}) h(\boldsymbol{\omega}) \right]^2 \\
&\leq \sup_{\|h\|=1} \int d\boldsymbol{\xi} (1 - \chi_R(\boldsymbol{\xi})) \left[\int d\boldsymbol{\omega} k(\boldsymbol{\xi}, \boldsymbol{\omega}) \right] \left[\int d\boldsymbol{\omega} k(\boldsymbol{\xi}, \boldsymbol{\omega}) (h(\boldsymbol{\omega}))^2 \right] \\
&\leq k_0 \sup_{\|h\|=1} \int d\boldsymbol{\xi} (1 - \chi_R(\boldsymbol{\xi}))(1 + |\boldsymbol{\xi}|)^{-1} \left[d\boldsymbol{\omega} k(\boldsymbol{\xi}, \boldsymbol{\omega}) (h(\boldsymbol{\omega}))^2 \right] \\
&\leq k_0 (1 + R)^{-1} \sup_{\|h\|=1} \int d\boldsymbol{\xi} \left[\int d\boldsymbol{\omega} k(\boldsymbol{\xi}, \boldsymbol{\omega}) (h(\boldsymbol{\omega}))^2 \right] \\
&\leq k_0 (1 + R)^{-1} \sup_{\|h\|=1} \int d\boldsymbol{\omega} (h(\boldsymbol{\omega}))^2 = k_0 (1 + R)^{-1}.
\end{aligned}$$

In addition $\chi_R K$, because of Theorem 3.2.2, is a Hilbert–Schmidt operator. Then, thanks to Eq. (3.2.23), K is compact, because the set of compact operators is a closed linear manifold in $B(L^2)$. Finally the fact that $K \in B(L^2) \cap B(L^\infty_\beta, L^\infty_{\beta+1})$, for $\beta \geq 0$, follows from Theorem 3.2.3 and $K \in C(L^2)$. □

We next consider the spectrum of L. Since in this section and the following ones we shall use several standard theorems on the perturbation of linear operators, for the sake of the reader we state them here and refer to the book of Kato[4] for the proofs. We denote by $K.(\ldots)$ the theorem $(\ldots)$ in Kato's book. In the statements below (where only the numbers of the equations and some symbols have been modified with respect to Ref. 4) $\mathcal{C}(\mathcal{X})$ means the set of closed operators from $\mathcal{X}$ to $\mathcal{X}$ and a holomorphic family of operators $T(\kappa)$ of type (A) is[4] such that $D(T(\kappa)) = D$ (independent of κ) and $T(\kappa)u$ is holomorphic in κ for every $u \in D$. We also recall the notion of relative compactness which is used in the statements below. Let T and A be operators with the same domain space $\mathcal{X}$ (but not necessarily with the same range space). Assume that $D(T) \subset D(A)$ and for any sequence $u_n \in D(T))$ with both u_n and Tu_n bounded, Au_n contains a convergent subsequence. Then A is said to be relatively compact with respect to T or simply T-compact.

Theorem K.IV.5.35. *The essential spectrum is conserved under a relatively compact perturbation. More precisely, let $T \in \mathcal{C}(\mathcal{X})$ and let A be T-compact. Then T and $T + A$ have the same essential spectrum.*

Theorem K.VII.2.6. *Let T be a closable operator from $\mathcal{X}$ to $\mathcal{Y}$ with $D(T) = D$. Let $T^{(n)}, n = 1, 2, \ldots$ be operators from $\mathcal{X}$ to $\mathcal{Y}$ with domains containing D and let there be constants $a, b, c \geq 0$ such that*

$$\| T^{(n)}u \| \leq c^{n-1}(a \| u \| + b \| Tu \|), \qquad (u \in D,\ n = 1, 2, \ldots). \tag{3.2.24}$$

Then the series

$$T(\kappa)u = Tu + \kappa T^{(1)}u + \kappa^2 T^{(2)}u + \cdots \qquad (u \in D) \tag{3.2.25}$$

defines an operator $T(\kappa)$ with domain D for $|\kappa| < 1/c$. If $|\kappa| < (b + c)^{-1}, T(\kappa)$ is closable and the closures $\tilde{T}(\kappa)$ for such κ form a holomorphic family of type (A).

Remark K.VII.2.7. The form of the condition (3.2.24) is so chosen as to be particularly convenient when $T^{(2)} = T^{(3)} = \cdots = 0$. In this case we can choose $c = 0$ if

$$\| T^{(1)}u \| \leq a \| u \| + b \| Tu \|, (u \in D) \ldots. \tag{3.2.26}$$

Theorem K.VII.1.8. *If $T(\kappa)$ is holomorphic in κ near $\kappa = 0$, any finite system of eigenvalues $\lambda_h(\kappa)$ of $T(\kappa)$ consists of branches of one or several analytic functions which have at most algebraic singularities near $\kappa = 0$. The same is true of the corresponding eigenprojections and eigennilpotents $Q_h(\kappa)$.*

We now prove

Theorem 3.2.5. *The spectrum $\sigma(L)$ of the operator L is made up of a discrete and an essential spectrum: the former is contained in the interval $(-\nu_0, 0]$, where $\nu_0 = \nu(0) = 4(2\pi)^{-1/2}$, while the latter coincides with $(-\infty, -\nu_0]$.*

Proof. This result follows from a particular case of Theorem K.IV. 5.35, i.e., Weyl's theorem on the perturbation of a self-adjoint operator[4] (the multiplication by $-\nu(|\boldsymbol{\xi}|)$) by a compact operator (K) and Theorem 3.2.1. □

Before ending this section we prove a result on the nonlinear term $\Gamma(h, h)$ or the corresponding bilinear operator $\Gamma(g, h)$ defined in Eq. (3.1.5):

Lemma 3.2.6. *The projection of $\Gamma(g, h)$ on the null space of L vanishes and there exists a constant $c \geq 0$ such that*

$$\| [\nu(\boldsymbol{\xi})]^{-1}\Gamma(g, h) \| \leq C \| h \| \| g \| \tag{3.2.27}$$

in L^∞_β for any $\beta \geq 0$.

Proof. The first part of the statement is obvious (because of the properties of $Q(f,g)$; the second part follows from the fact that $|g| \leq \| g \| (1+|\boldsymbol{\xi}|^2)^{-\beta/2}$and hence for any piece Γ_i $(i = 1-4)$ in which we can split $\Gamma(= \Gamma_1 + \Gamma_2 - \Gamma_3 - \Gamma_4)$ we have

$$\| [\nu(\boldsymbol{\xi})]^{-1}\Gamma_i(g,h) \| \leq \| R^{-1}[\nu(\boldsymbol{\xi})]^{-1}Q(R(1+|\boldsymbol{\xi}|^2)^{-\beta/2},$$
$$R(1+|\boldsymbol{\xi}|^2)^{-\beta/2}) \| \| h \| \| g \| \leq \| (1+|\boldsymbol{\xi}|^2)^{-\beta/2} \| \| h \| \| g \| = C \| h \| \| g \| \tag{3.2.28}$$

where we have noted that, e.g.,

$$(1+|\boldsymbol{\xi}'|^2)^{-\beta/2}(1+|\boldsymbol{\xi}'_*|^2)^{-\beta/2} \leq (1+|\boldsymbol{\xi}'|^2+|\boldsymbol{\xi}'_*|^2)^{-\beta/2} \leq (1+|\boldsymbol{\xi}|^2+|\boldsymbol{\xi}_*^2)^{-\beta/2}$$
$$\leq (1+|\boldsymbol{\xi}|^2)^{-\beta/2} \tag{3.2.29}$$

and this concludes the proof. □

3.3 Some Spectral Properties

We want to look for a solution of the Cauchy problem of Eq. (3.1.3) in $\Re^3$ or in a periodic box. As a preliminary step we consider the *linearized Boltzmann equation*, obtained by neglecting the nonlinear term in Eq. (3.1.3):

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial h}{\partial \mathbf{x}} = Lh. \tag{3.3.1}$$

We first consider the case of $\Re^3$ and use the Fourier transform in $\mathbf{x}$:

$$\hat{h}(\mathbf{k},\boldsymbol{\xi},t) = (2\pi)^{-3/2}\int h(\mathbf{x},\boldsymbol{\xi},t)e^{-i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}. \tag{3.3.2}$$

Then $\hat{h}$ satisfies

$$\frac{\partial \hat{h}}{\partial t} + i\boldsymbol{\xi}\cdot\mathbf{k}\hat{h} = L\hat{h} \tag{3.3.3}$$

or, for short,

$$\frac{\partial \hat{h}}{\partial t} = B(\mathbf{k})\hat{h} \tag{3.3.4}$$

where

$$B(\mathbf{k}) = L - i\boldsymbol{\xi}\cdot\mathbf{k}I = K - \sigma(\boldsymbol{\xi};\mathbf{k})I. \tag{3.3.5}$$

Here $\sigma(\boldsymbol{\xi};\mathbf{k})$ is a function given by

$$\sigma(\boldsymbol{\xi};\mathbf{k}) = \nu(|\boldsymbol{\xi}|) + i\mathbf{k}\cdot\boldsymbol{\xi}. \tag{3.3.6}$$

Let us consider $\mathbf{k}$ as a parameter so that we deal with $L^2(\Re^3)$ for the moment. We want to study the semigroup $T(t;\mathbf{k})$ generated by $B(\mathbf{k})$. The first result is the following:

Lemma 3.3.1. *The operator $B(\mathbf{k})$ with domain $D(B(\mathbf{k})) = \{f(\boldsymbol{\xi}) : f \in L^2, |\boldsymbol{\xi}|f \in L^2\}$ is an unbounded operator with domain dense in L^2, generating a strongly continuous semigroup $T(t;\mathbf{k})$ with*

$$||T(t;\mathbf{k})|| \leq 1. \tag{3.3.7}$$

Proof. The multiplication operator $S(\mathbf{k}) = -\sigma(\boldsymbol{\xi};\mathbf{k})I$ generates the strongly continuous semigroup

$$U(t;\mathbf{k}) = \exp[-\sigma(\boldsymbol{\xi};\mathbf{k})t]I. \tag{3.3.8}$$

$B(\mathbf{k})$, being a compact perturbation of $S(\mathbf{k})$, generates a strongly continuous semigroup $T(t;\mathbf{k})$ in L^2. Estimate (3.3.7) follows because L is self-adjoint, non-positive and $-i\mathbf{k}\cdot\boldsymbol{\xi}I$ antisymmetric. □

We note that this theorem establishes the existence of a unique solution of the Cauchy problem for the linearized Boltzmann equation in L^2; in fact if the initial condition is $h(0) = h_0, h(t) = T(t)h_0$ where $T(t)h_0$ is the inverse Fourier transform of $T(t;\mathbf{k})\hat{h}_0$, where $\hat{h}_0$ is the Fourier transform of h_0.

We shall now study the asymptotic behavior of $T(t;\mathbf{k})$ when $t \to \infty$. To this end it is useful to recall the representation of $T(t;\mathbf{k})$ in terms of its Laplace transform $R(\lambda;\mathbf{k})$ which equals the resolvent of $B(\mathbf{k})$:

$$R(\lambda;\mathbf{k}) = (\lambda I - B(\mathbf{k}))^{-1}. \tag{3.3.9}$$

The above-mentioned representation reads as follows:

$$T(t;\mathbf{k})h = \frac{1}{2\pi i}\ \text{s-}\lim_{\delta\to\infty}\int_{\gamma-i\delta}^{\gamma+i\delta} \exp(\lambda t)R(\lambda;\mathbf{k})h d\lambda \tag{3.3.10}$$

$(t, \gamma > 0, h \in D(B(\mathbf{k}))$. This is a formal relation that we shall presently justify. To this end, we need a few results concerning the operator $R(\lambda;\mathbf{k})$. We shall write $\text{Re}\lambda$ and $\text{Im}\lambda$ for the real and imaginary parts of a complex number λ. The first result is given in

Lemma 3.3.2. *For any fixed $\mathbf{k}$, the operator $R(\lambda;\mathbf{k})$ is an analytic function of λ in the half-plane $\text{Re}\lambda \geq -\nu_0 + \epsilon$ $(\epsilon > 0)$ with the exception of a finite number of poles of finite multiplicity $\{\lambda_j(\mathbf{k})\}$. These poles satisfy the following conditions:*

1) $\text{Re}\lambda_j(\mathbf{k}) \leq 0$ *and* $\text{Re}\lambda_j(\mathbf{k}) = 0$ *implies* $\lambda = k = 0$.

2) $|\text{Im}\lambda_j(\mathbf{k})| \leq c(\epsilon)$.

Proof. $R(\lambda;\mathbf{k})$ can be expressed as follows:

$$R(\lambda;\mathbf{k}) = (\lambda I - B(\mathbf{k}))^{-1} = (\lambda I - S(\mathbf{k}) - K)^{-1} = (I - \overline{R}(\lambda;\mathbf{k})K)^{-1}\overline{R}(\lambda;\mathbf{k}) \tag{3.3.11}$$

where $\overline{R}(\lambda;\mathbf{k}) = (\lambda I - S(\mathbf{k}))^{-1} = (\lambda + \sigma(\boldsymbol{\xi};\mathbf{k}))^{-1}I$ is the multiplication by a function, analytic in λ for $\lambda > -\nu$. Since K is compact, $(I - \overline{R}(\lambda;\mathbf{k})K)^{-1}$ exists as a bounded operator with the exception of countably many isolated points. Eq. (3.3.11) shows that $R(\lambda;\mathbf{k})$ has the same property. In addition the points where $R(\lambda;\mathbf{k})$ is unbounded are those for which there is a function $\psi \neq 0$ such that $\overline{R}(\lambda;\mathbf{k})K\psi = \psi$ or

$$B(\mathbf{k})\psi = \lambda\psi. \tag{3.3.12}$$

Condition 1) follows from a direct calculation of $\mathrm{Re}\lambda$ from this equation. Further the compactness of K implies that the eigenvalues can only accumulate near the line $\mathrm{Re}\lambda = -\nu_0$; this implies that for $\mathrm{Re}\lambda \geq -\nu_0 + \epsilon$ ($\epsilon > 0$) there is only a finite number of eigenvalues and condition 2) holds. □

Further information on $\overline{R}(\lambda;\mathbf{k})$ is provided by

Lemma 3.3.3. *For any* $\epsilon > 0$ $\| K\overline{R}(\lambda;\mathbf{k}) \| \to 0$ *for* $|\mathbf{k}| \to \infty$ *, uniformly for* $\mathrm{Re}\lambda \geq -\nu_0 + \epsilon$ *and* $\| K\overline{R}(\lambda;\mathbf{k}) \| \to 0$ $(|\mathrm{Im}\lambda| \to \infty)$ *uniformly for* $\mathrm{Re}\lambda \geq -\nu_0 + \epsilon$ *and* $\mathbf{k}$ *such that* $|\mathbf{k}| < k_0$ *, for any fixed* $k_0 > 0$.

Proof. In fact, if $\chi_R(\boldsymbol{\xi})$ is the characteristic function of the ball $|\boldsymbol{\xi}| \leq R$, then the square-integrability of the kernel of K implies (Schwarz's inequality):

$$\| K\chi_R\overline{R}(\lambda;\mathbf{k}) \| \leq C\Big(\int_{|\boldsymbol{\xi}|<R} |\lambda + i\mathbf{k}\cdot\boldsymbol{\xi} + \nu(\boldsymbol{\xi})|^{-2} d\boldsymbol{\xi}\Big)^{1/2} \tag{3.3.13}$$

The last integral can be subdivided into two contributions, one extended to the subset $|\mathrm{Im}\lambda + \mathbf{k}\cdot\boldsymbol{\xi}| \leq |\mathbf{k}|\delta$ ($\delta > 0$) and the other to the complement of this subset in $|\boldsymbol{\xi}| < R$. The first subset is not larger than a parallelepipedon with two edges of length R and the third of length 2δ, so that its measure is less than $2R^2\delta$ and in it the integrand is less than ϵ^{-2}, while the second set has measure less than $4\pi R^3/3$ and the integrand is certainly not larger than $(|\mathbf{k}|\delta)^{-2}$. Hence

$$\| K\chi_R\overline{R}(\lambda;\mathbf{k}) \| \leq CR[\epsilon^{-2}\delta + R(|\mathbf{k}|\delta)^{-2}]^{1/2}. \tag{3.3.14}$$

If we choose $\delta = (R/|\mathbf{k}|)^{2/3}$ we have

$$\| K\chi_R\overline{R}(\lambda;\mathbf{k}) \| \leq C(\epsilon)R^{4/3}|\mathbf{k}|^{-1/3}. \tag{3.3.15}$$

On the other hand Eq. (3.2.23) gives (thanks to $\| \overline{R}(\lambda;\mathbf{k}) \| \leq \epsilon^{-1}$):

$$\| K(1-\chi_R)\overline{R}(\lambda;\mathbf{k}) \| \leq C\epsilon^{-1}(1+R^2)^{-1/2}. \tag{3.3.16}$$

If we put together the two estimates and choose $R = |\mathbf{k}|^{1/6}$, we obtain the first statement of the lemma. To prove the second one, let $|\mathrm{Im}\lambda| \geq 2k_0\mathrm{R}$. Then $|\mathrm{Im}\lambda + \mathbf{k}\cdot\boldsymbol{\xi}| \geq |\mathrm{Im}\lambda|/2$ whenever $|\mathbf{k}| \leq k_0$ and $|\boldsymbol{\xi}| \leq R$, so that for $\mathrm{Re}\lambda > -\nu_0 + \epsilon$,

$$\| K\chi_R\overline{R}(\lambda;\mathbf{k}) \| \leq C(4\pi R^3/3)^{1/2}(\epsilon^2 + |\mathrm{Im}\lambda|^2/4)^{1/2}. \tag{3.3.17}$$

We can now choose here and in (3.3.16) $R = |\mathrm{Im}\lambda|^{2/5}$, which is possible for $|\mathrm{Im}\lambda| \geq (2k_0)^{5/3}$, since we have chosen $|\mathrm{Im}\lambda| \geq 2k_0R$. □

To proceed further, we need

Lemma 3.3.4. *For any* $\gamma = \mathrm{Re}\lambda > -\nu_0$*, we have*

$$\int_{\gamma-i\delta}^{\gamma+i\delta} \| \overline{R}(\lambda;\mathbf{k})h \|^2 \, d\lambda \leq \pi(\gamma+\nu_0)^{-1} \| h \|^2 . \tag{3.3.18}$$

Proof. If we recall the representation

$$\overline{R}(\lambda;\mathbf{k}) = \int_0^\infty \exp(-\lambda t) U(t;\mathbf{k}) dt \qquad (\mathrm{Re}\lambda > -\nu_0) \tag{3.3.19}$$

and denote by $\chi_+(t)$ the Heaviside step function, we have

$$\overline{R}(\lambda;\mathbf{k}) = (2\pi)^{-1/2} \int_0^\infty \exp(-\lambda t)[(2\pi)^{1/2} U(t;\mathbf{k})\chi_+(t)] dt \tag{3.3.20}$$

($\mathrm{Re}\lambda > -\nu_0$) which shows that, for a fixed value of $\mathrm{Re}\lambda$, $\overline{R}(\lambda;\mathbf{k})$ is the Fourier transform (in the variable $\mathrm{Im}\lambda$) of the function of t,

$$(2\pi)^{1/2} U(t;\mathbf{k})\chi_+(t) \exp[-(\mathrm{Re}\lambda)t].$$

Then Parseval's equality gives

$$\int_{\gamma-i\delta}^{\gamma+i\delta} \| \overline{R}(\lambda;\mathbf{k})h \|^2 \, d\lambda = 2\pi \int_0^\infty \| U(t;\mathbf{k})h \|^2 \exp(-2\gamma t) dt. \tag{3.3.21}$$

Since $\| U(t;\mathbf{k})h \| \leq \| h \| \exp(-\nu_0 t)$, the lemma follows. □

According to Lemma 3.3.2, at the right of the line $\mathrm{Re}\lambda = -\nu_0 + \epsilon$ ($\epsilon > 0$) there is only a finite number of eigenvalues λ_j and they can be numbered as

$$\mathrm{Re}\lambda_1 \geq \mathrm{Re}\lambda_2 \geq \mathrm{Re}\lambda_3 \geq \cdots \mathrm{Re}\lambda_r \geq -\nu_0 + \epsilon. \tag{3.3.22}$$

We shall denote by P_j the projector on the eigenspace of $B(\mathbf{k})$ corresponding to the eigenvalue λ_j. If the eigenvalue is not simple, we denote by m_j its multiplicity. In this case we only know that $B(\mathbf{k}) - \lambda_j I$ is nilpotent of rank m_j on the functions $P_j f$ obtained by projecting on the associated subspace of dimension m_j, but, in general, the functions of this subspace are not eigenfunctions of $B(\mathbf{k})$, because the associated matrix will in general be a "Jordan block". We remark that, in principle, we should write $\lambda_j(\mathbf{k}), P_j(\mathbf{k}), \ldots$ in place of $\lambda_j, P_j, \ldots$, but we shall do this only after the proof of Theorem 3.3.5, when we shall discuss the dependence of these quantities upon $\mathbf{k}$.

Let us denote by P the projector on the subspace spanned by all the P_j, i.e.,

$$P = \sum_{j=1}^{r} P_j \tag{3.3.23}$$

We can prove the following

Theorem 3.3.5. *Assume (for a given* ϵ*) that* $\mathrm{Re}\lambda_j \neq -\nu_0 + \epsilon$*. Then*

$$T(t;\mathbf{k})P = \sum_{j=1}^{r}(\exp(\lambda_j t)(P_j + \sum_{k=1}^{m_j}\frac{t^k}{k!}Q_j^k), \tag{3.3.24}$$

$$\| T(t;\mathbf{k})(I-P) \| \leq C\exp[(-\nu_0+\epsilon)t]. \tag{3.3.25}$$

Here the Q_j *are nilpotent operators associated with the Jordan block corresponding to the eigenvalue* λ_j *and* C *is a constant independent of* $\mathbf{k}$*. More precisely (see Kato*[4]*, p.* 181*) they are the residue of* $-(\lambda-\lambda_j)R(\lambda;\mathbf{k})$ *at a multiple pole of* $R(\lambda;\mathbf{k})$*.*

Proof. The inverse Laplace transform for $T(t;\mathbf{k})$ is given by Eq. (3.3.10), which is no longer formal now, because of the estimate (3.2.18) . Further, we have

$$R(\lambda;\mathbf{k}) = (\lambda I - B(\mathbf{k}))^{-1} = (\lambda I - S(\mathbf{k}) - K)^{-1} = \overline{R}(\lambda;\mathbf{k})(I - K\overline{R}(\lambda;\mathbf{k}))^{-1} \tag{3.3.26}$$

and hence

$$R(\lambda;\mathbf{k}) = \overline{R}(\lambda;\mathbf{k}) + R(\lambda;\mathbf{k})K\overline{R}(\lambda;\mathbf{k}) \tag{3.3.27}$$

and using again Eq. (3.26) in the right-hand side of Eq. (3.3.27):

$$R(\lambda;\mathbf{k}) = \overline{R}(\lambda;\mathbf{k}) + \overline{R}(\lambda;\mathbf{k})[I - K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k}). \tag{3.3.28}$$

Then

$$\begin{aligned} &T(t;\mathbf{k})h \\ &= U(t;\mathbf{k})h + \frac{1}{2\pi i}\text{s-}\lim_{\delta\to\infty}\int_{\gamma-i\delta}^{\gamma+i\delta}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda \end{aligned} \tag{3.3.29}$$

($\gamma > 0$). We now shift the integration line from $\mathrm{Re}\lambda > 0$ to $\mathrm{Re}\lambda = -\nu_0 + \epsilon$. Since the integrand has only poles in $\mathrm{Re}\lambda \geq -\nu_0 + \epsilon$, we have

$$\begin{aligned} &\int_{\gamma-i\delta}^{\gamma+i\delta}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda \\ &= 2\pi i\sum_{j=1}^{r}\mathrm{Res}_{\lambda=\lambda_j}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda \\ &\quad + \int_{-\nu_0+\epsilon-i\delta}^{-\nu_0+\epsilon+i\delta}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda + Z \end{aligned} \tag{3.3.30}$$

where

$$Z = \Big(\int_{-\nu_0+\epsilon-i\delta}^{\gamma+i\delta} - \int_{\nu_(0)+\epsilon+i\delta}^{\gamma-i\delta}\Big)\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda. \tag{3.3.31}$$

In order to evaluate the residues in Eq. (3.2.30), we first remark that, because of (3.3.28), they are the same as the residues of $R(\lambda;\mathbf{k})$ (since λ_j is in the resolvent set of S). Then, because of the expansion of the resolvent (Kato[4], p. 181), we get the following result:

$$\begin{aligned}&\mathrm{Res}_{\lambda=\lambda_j}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})\\&=\mathrm{Res}_{\lambda=\lambda_j}\exp(\lambda t)R(\lambda;\mathbf{k})=(\exp(\lambda_j t)(P_j+\sum_{k=1}^{m_j}\frac{t^k}{k!}Q_j^k)\end{aligned}\tag{3.3.32}$$

Next, because of Lemma 3.3.3, which also implies that $[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}$ is bounded for $\mathrm{Im}\lambda$ sufficiently large, and since for $\mathrm{Re}\lambda>-\nu_0$,

$$\|\overline{R}(\lambda;\mathbf{k})\|=\|(\lambda+i\mathbf{k}\cdot\boldsymbol{\xi}+\nu(\boldsymbol{\xi}))^{-1}I\|\le(\mathrm{Re}\lambda+\nu_0)^{-1},\tag{3.3.33}$$

$\| Z \|\to 0$ when $\delta\to\infty$. Finally, since (by assumption) there are no eigenvalues on $\mathrm{Re}\lambda=-\nu_0+\epsilon$, $\|[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}\|\le C$ on any compact set of that line and, because of the second statement of Lemma 3.3.3, on the entire line as well, with C independent of $\mathbf{k}$. Then, for any $h,g\in L^2$:

$$\begin{aligned}&\Big|\Big(\int_{-\nu 0+\epsilon-i\delta}^{-\nu_0+\epsilon+i\delta}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})hd\lambda,g\Big)\Big|\\&\le\exp[-(\nu_0-\epsilon)t]\int_{-\delta}^{\delta}|(\overline{R}(-\nu_0+\epsilon+i\tau;\mathbf{k})[I-K(-\nu_0+\epsilon+i\tau;\mathbf{k})]^{-1}\\&\qquad\qquad\times K\overline{R}(-\nu_0+\epsilon+i\tau;\mathbf{k})d\tau,g)|\\&\le C\|K\|\exp[-(\nu_0-\epsilon)t]\int_{-\delta}^{\delta}\|\overline{R}(-\nu_0+\epsilon+i\tau;\mathbf{k})h\|\|\overline{R}(-\nu_0+\epsilon-i\tau;\mathbf{k})g\|d\tau.\end{aligned}\tag{3.3.34}$$

Then, because of Eq. (3.3.18) the last integral is bounded by $\pi(\gamma+\nu_0)^{-1}\parallel h\parallel\parallel g\parallel$. This implies not only the convergence (for $\delta\to\infty$) of the operator

$$\int_{-\nu 0+\epsilon-i\delta}^{-\nu_0+\epsilon+i\delta}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})d\lambda$$

in the weak operator topology, but also that its limit satisfies:

$$\begin{aligned}&\Big\|\int_{-\nu_0+\epsilon-i\infty}^{-\nu_0+\epsilon+i\infty}\exp(\lambda t)\overline{R}(\lambda;\mathbf{k})[I-K\overline{R}(\lambda;\mathbf{k})]^{-1}K\overline{R}(\lambda;\mathbf{k})\Big\|\\&\qquad\le C\exp[-(\nu_0-\epsilon)t]\quad(t\in\Re_+).\end{aligned}\tag{3.3.35}$$

If we combine the estimates we obtain the theorem. □

This important result was first obtained by Ukai[9] and is a key result for the treatment of the study of the asymptotic behavior of the linearized Boltzmann equation and of the existence theory for the weakly nonlinear Boltzmann equation.

The next step is due to Ellis and Pinsky[2] (see also McLennan[6] and Arsen'ev[1]):

Theorem 3.3.6. *One can find functions $\mu_j(|\mathbf{k}|) \in C^\infty([-k_0, k_0])$, $j = 0, 1, \ldots, 4$, and positive numbers k_0 and σ_0 ($< \nu_0$) such that*

a) *for any $\mathbf{k} \in \Re^3$ with $|\mathbf{k}| \leq k_0$, there are five eigenvalues λ_j given by $\lambda_j(\mathbf{k}) = \mu_j(|\mathbf{k}|)$ where*

$$\mu_j(|\mathbf{k}|) = i\mu_j^{(1)}|\mathbf{k}| - \mu_j^{(2)}|\mathbf{k}|^2 + O(|\mathbf{k}|^3) \qquad (\mathbf{k}| \to 0) \tag{3.3.36}$$

and $\mu_j^{(1)} \in \Re$ and $\mu_j^{(2)} \in \Re_+$. In addition

$$P_j(\mathbf{k}) = P_j^{(0)}(\mathbf{k}/|\mathbf{k}|) + |\mathbf{k}|P_j^{(1)}(\mathbf{k}/|k|),$$

$$Q_j(\mathbf{k}) = 0, \tag{3.3.37}$$

for $j = 1, 2, \ldots, 5$, where $P_j^{(0)}$ are orthogonal projectors and

$$P_0 = \sum_{j=1}^{5} P_j^{(0)}(\mathbf{k}/|\mathbf{k}|) \tag{3.3.38}$$

does not depend upon $\mathbf{k}/|\mathbf{k}|$ and projects on the five-dimensional eigenspace of the collision invariants.

b) *for any $\mathbf{k} \in \Re^3$ with $|\mathbf{k}| > k_0$, there are no eigenvalues with $\mathrm{Re}\lambda \leq -\sigma_0$.*

Proof. The fact that the eigenvalues only depend upon $|\mathbf{k}|$ follows from the fact that the linearized collision operator commutes with any rotation $\mathcal{R}$ of $\Re^3$ and $\mathcal{R}\mathbf{k} \cdot \mathcal{R}\boldsymbol{\xi} = \mathbf{k} \cdot \boldsymbol{\xi}$; hence if $\varphi(\boldsymbol{\xi}; \mathbf{k})$ is an eigenfunction corresponding to an eigenvalue λ, then $\varphi(\mathcal{R}\boldsymbol{\xi}; \mathcal{R}\mathbf{k})$ is an eigenfunction corresponding to the same eigenvalue, which thus can only depend on $|\mathbf{k}|$. Please note that the eigenfunction itself and the corresponding projector do not, generally speaking, depend on $|\mathbf{k}|$ alone, contrary to what is stated sometimes. We can now replace $\mathbf{k}$ by $\kappa\mathbf{e}$ (where $\mathbf{e} = k/\kappa$ is a unit vector and κ is $\pm|\mathbf{k}|$) and look for a solution depending analytically on κ, according to Theorem K.VI.1.8 on the analytic perturbations of linear operators[4] in L^2, which, according to Theorem K.VII.2.6 and Remark K.VII.2.7, applies here, because there is a constant M, such that $\| \mathbf{e} \cdot \boldsymbol{\xi} h \| \leq M(\| h \| + \| Lh \|)$; thus the eigenvalues are analytic functions of κ. In particular, since for $\kappa = 0$ there are five eigenfunctions corresponding to the zero eigenvalue, for a sufficiently small κ there will be five eigenvalues (which may be distinct or not) whose expression will be given by Eq. (3.3.36). In order to show that $\mu_j^{(1)} \in \Re$ we remark that the operator $B(\mathbf{k})$ is invariant with respect to the product $\mathcal{CP}$ of the operations $\mathcal{P}$ of changing κ into $-\kappa$ and $\mathcal{C}$ of taking the complex conjugate; the same invariance applies to the eigenvalues and this proves that $\mu_j^{(1)} \in \Re$. To prove that $\mu_j^{(2)} \in \Re_+$, we remark that if ψ_j are the normalized eigenfunctions , then $\psi_j(\kappa) = \psi_j(0) + \kappa\psi_j'(0) + \kappa^2\psi_j 0)/2 + \cdots$ and hence:

$$\begin{aligned}\lambda_j \quad &= (\psi_j, B(\mathbf{k})\psi_j) = (\psi_j, L\psi_j) - i\kappa(\psi_j, \mathbf{e}\cdot\boldsymbol{\xi}\psi_j) \\ = \quad &(\psi_j(0), L\psi_j(0)) + \kappa(\psi_j'(0), L\psi_j(0)) + \kappa(\psi_j(0), L\psi_j'(0)) \\ &+\kappa^2(\psi_j'(0), L\psi_j'(0)) + (\kappa^2/2)(\psi_j(0), L\psi_j''(0)) \\ &+(\kappa^2/2)(\psi_j''(0), L\psi_j(0)) - i\kappa(\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0)) \\ &-i\kappa^2(\psi_j'(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0)) - i\kappa^2(\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j'(0)) + O(\kappa^3).\end{aligned} \tag{3.3.39}$$

Since, however, the functions $\psi_j(0)$ are collision invariants, many of the scalar products above are zero and we are left with:

$$\begin{aligned}\lambda_j \quad &= -i\kappa(\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0)) + \kappa^2(\psi_j'(0), L\psi_j'(0)) \\ &-i\kappa^2[(\psi_j'(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0)) + (\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j'(0))] + O(\kappa^3).\end{aligned} \tag{3.3.40}$$

We now remark that the term in square brackets is real (since the factor $\mathbf{e}\cdot\boldsymbol{\xi}$ is self-adjoint, the two terms in the bracket are complex conjugate of each other); but this would imply that λ_j is not invariant with respect to $\mathcal{CP}$, as must be by the above argument, unless the term in square brackets vanishes. Our final expression for λ_j will thus be

$$\lambda_j = -i\kappa(\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0)) + \kappa^2(\psi_j'(0), L\psi_j'(0)) + O(\kappa^3). \tag{3.3.41}$$

This now coincides with Eq. (3.3.36) and indeed the coefficient of κ^2 is negative because of the properties of the linearized collision operator. (Note that $\psi_j'(0)$ cannot be a collision invariant because $L\psi_j'(0) = i[\mathbf{e}\cdot\boldsymbol{\xi} - (\psi_j(0), \mathbf{e}\cdot\boldsymbol{\xi}\psi_j(0))]\psi_j(0) \neq 0$.)

Finally since the spectrum of $B(\mathbf{k})$ is discrete and depends analytically on κ, we can obtain (3.3.37) and (3.3.38); the latter is obvious and the former follows from the fact that analyticity allows us to take a purely imaginary κ and obtain a self-adjoint operator $B(\kappa\mathbf{e})$, for which diagonalization is possible (without Jordan blocks).

In order to prove *b*), we first prove that for any $\delta > 0$, there exists $k_0 = k_0(\delta)$ such that whenever $|\mathbf{k}| < k_0$ and λ is in the discrete spectrum of $B(\mathbf{k})$, the following holds:

$$\mathrm{Re}\lambda \geq -\sigma_1 \qquad \text{implies} \qquad |\mathrm{Im}\lambda| \leq \delta, \tag{3.3.42}$$

$$\mathrm{Re}\lambda \geq -\mu/2 \qquad \text{implies} \qquad |\lambda| \leq \delta \tag{3.3.43}$$

where $-\mu$ is, among the nonzero eigenvalues of L, the closest to the origin, while σ_1 is any real number between μ and $\nu(0)$.

In fact if (3.3.42) is violated, then, for some $\delta > 0$, there exists a sequence of real numbers $\{k_n\}$ converging to zero, a corresponding sequence of eigenvalues $\{\lambda_n\}$ and a sequence $\{h_n\}$ of L^2-functions (with unit norm) such that

$$B(k_n)h_n = \lambda_n h_n, \tag{3.3.44}$$

$$|\mathrm{Im}\lambda_n| > \delta, \qquad \mathrm{Re}\lambda_n \geq -\sigma_1. \tag{3.3.45}$$

Let us show that $\overline{\lim}|\mathrm{Im}\lambda_n| < +\infty$. In fact, Eq. (3.3.44) states that

$$Kh_n = (\lambda_n + \nu(\boldsymbol{\xi}) + ik_n \cdot \boldsymbol{\xi})h_n. \tag{3.3.46}$$

Since K is compact, we may assume that $Kh_n \to g$ in L^2, by choosing a subsequence, if necessary. Now if $|\mathrm{Im}\lambda_n|$ converged to $+\infty$, we would have, from (3.3.46), that h_n should converge to zero, in contradiction to $\| h_n \|= 1$. Hence for some C, there are infinitely many indices n such that $\delta < |\mathrm{Im}\lambda_n| \leq$C. Since $0 \geq \mathrm{Re}\lambda_n \geq -\sigma_1$, we may extract a convergent subsequence $\{\lambda_n\}$ with limit λ such that $\mathrm{Im}\lambda \neq 0$. Taking the limit in Eq. (3.3.46), we obtain that h_n has a nonzero limit in L^2, which satisfies

$$Kh = (\lambda + \nu(\boldsymbol{\xi}))h \tag{3.3.47}$$

and this, because of the self-adjointness of L implies $\mathrm{Im}\lambda = 0$, a contradiction which proves (3.3.42). To prove (3.3.43), we proceed in a similar way: if (3.3.43) is violated, then, for some $\delta > 0$, there exists a sequence of real numbers $\{k_n\}$ converging to zero, a corresponding sequence of eigenvalues $\{\lambda_n\}$ and a sequence $\{h_n\}$ of L^2-functions (with unit norm) such that Eq. (3.3.44) holds with

$$-\mu/2 \leq \mathrm{Re}\lambda_n \leq -\delta. \tag{3.3.48}$$

Because of (3.3.42), that we have just proved, $|\mathrm{Im}\lambda_n| \leq \delta$ and we can extract a subsequence $\{\lambda_n\}$ converging to a real λ with $-\mu/2 \leq \lambda \leq -\delta$. Taking now the limit in Eq. (3.3.46), we obtain, as above, Eq. (3.3.47). Since $\lambda \neq 0$ and L is self-adjoint, h must be orthogonal to the null space of L; but this would imply, by the definition of $\mu, \lambda < \mu$, a contradiction that proves (3.3.43).

In order to finish the proof, let us show that there is a neighborhood $\mathcal{N}_1 \times \mathcal{N}_2$ of the origin in $\Re \times C$, such that if $\lambda = \lambda(\kappa\mathbf{e})$ ($\mathbf{e} \in S^2$) with $\kappa \in \mathcal{N}_1$ and $\lambda \in \mathcal{N}_2$, then λ is one of the five eigenvalues discussed in part a) of the theorem. Let us define $H = \nu^{-1}K - \nu^{-1/2}P_\nu\nu^{1/2}$, where P_ν projects on the subspace spanned by the eigenfunctions of $\nu^{-1/2}K\nu^{-1/2}$ corresponding to a unit eigenvalue. Clearly, H is compact. Also H cannot have $\lambda = 1$ as eigenvalue, because otherwise there would be a function h such that $Hh = h$ or

$$Lh = \nu^{1/2}P_\nu\nu^{1/2}h. \tag{3.3.49}$$

Then projecting upon the null space of L we obtain that $\nu^{1/2}h$ is orthogonal to the range of P_ν. Since P_ν is a projector, this implies that $P_\nu(\nu^{1/2}h) = 0$ and, because of Eq. (3.3.49), h must be in the null space of L; this together with $P_\nu(\nu^{1/2}h) = 0$ implies $h = 0$ and $\lambda = 1$ is not an eigenvalue of H.

Let us now prove that there exists a neighborhood $\mathcal{N}_1 \times \mathcal{N}_2$ of the origin in $\Re \times C$ such that for $(\kappa, \lambda) \in \mathcal{N}_1 \times \mathcal{N}_2$, the operator $I - (\nu + i\mathbf{k} \cdot \boldsymbol{\xi} + \lambda)^{-1}\nu H$ is invertible. The operator $(\nu + i\mathbf{k} \cdot \boldsymbol{\xi} + \lambda)^{-1}\nu H$, being the product of a bounded operator by a compact operator is compact. By the Fredholm alternative it is then sufficient to prove that there is no function h such that

$$h = (\nu + i\mathbf{k}\cdot\boldsymbol{\xi} + \lambda)^{-1}\nu H h \tag{3.3.50}$$

for k and λ sufficiently small. Assume the contrary, i.e., that there exist sequences $\{k_n\}, \{\lambda_n\}$ converging to zero and $\{h_n\}$ ($\| h_n \| = 1$) satisfying (3.3.50); since H is compact and the factor multiplying it in (3.3.50) is bounded uniformly and converges strongly to 1 when $\mathbf{k}$ and λ converge to zero, we have that h_n converges to some g (with $\| g \| = 1$) that satisfies the limiting equation $Hg = g$. We have shown, however, that $Hg = g$ implies $g = 0$ and the invertibility of $I - (\nu + i\mathbf{k}\cdot\boldsymbol{\xi} + \lambda)^{-1}\nu H$ is proved.

We are now ready to attack the original problem $B(\mathbf{k})h = \lambda h$ by rewriting it in terms of H:

$$\nu H h + \nu^{1/2} P_\nu \nu^{1/2} h = (\nu + i\mathbf{k}\cdot\boldsymbol{\xi} + \lambda)h \tag{3.3.51}$$

or

$$h = [I - (\nu + i\mathbf{k}\cdot\boldsymbol{\xi} + \lambda)^{-1}\nu H]^{-1}(\nu + i\mathbf{k}\cdot\boldsymbol{\xi} + \lambda)^{-1}\nu^{1/2} P_\nu \nu^{1/2} h. \tag{3.3.52}$$

This form of the problem gives h once $P_\nu \nu^{1/2} h$ is known; and since P_ν has a finite range, we can compute $P_\nu \nu^{1/2} h$ by solving a system of five linear algebraic equations in five unknowns, by simply projecting Eq. (3.3.52). The determinant of the system will be some analytic function of λ and κ , $D(\lambda, \kappa)$. For $\kappa = 0$, Eq. (3.3.51) is equivalent to $Lh = \lambda h$ and hence in a neighborhood of $\lambda = 0$ there will be only a fivefold degenerate zero of $D(\lambda, 0)$; by continuity, for a sufficiently small κ, there will be just five zeroes of $D(\lambda, \kappa)$ in a neighborhood of the origin in $\Re \times C$, as was to be shown. This, when combined with (3.3.42) and (3.3.43) gives part b) of Theorem 3.3.6. $\square$

From this theorem and the previous one, we obtain the following

Corollary 3.3.7. *There is a constant $C \geq 0$ such that*

a) *for any $\mathbf{k} \in \Re^3$ with $|\mathbf{k}| \leq k_0$ (where k_0 is the same as in Theorem 3.3.6):*

$$T(t; \mathbf{k}) = \sum_{j=0}^{n+1} (\exp(\mu_j(|\mathbf{k}|)t) P_j(K) + V(t, \mathbf{k}), \tag{3.3.53}$$

$$\| V(t; \mathbf{k}) \| \leq C \exp[(-\nu_0 + \epsilon)t] \qquad (t \geq 0); \tag{3.3.54}$$

b) *for any $\mathbf{k} \in \Re^3$ with $|\mathbf{k}| > k_0$,*

$$\| T(t; \mathbf{k}) \| \leq C \exp[(-\nu_0 + \epsilon)t](t \geq 0). \tag{3.3.55}$$

The constant C in Eqs. (3.3.54) *and* (3.3.55) *is independent of* $\mathbf{k}$ *because this is guaranteed by Theorem* 3.3.5.

3.4 The Asymptotic Behavior of the Solution of the Cauchy Problem for the Linearized Boltzmann Equation

We can now establish a decay estimate for $T(t)$, the semigroup generated by the operator $B = L - \boldsymbol{\xi} \cdot \partial/\partial\mathbf{x}$ in ordinary space. To this end we introduce the L^2-Sobolev space $H^s(\Re^3{}_{\mathbf{x}})$ and define

$$H_s = L^2(\Re^3{}_{\boldsymbol{\xi}}, H^s(\Re^3{}_{\mathbf{x}})), \qquad L^{q,2} = L^2(\Re^3{}_{\boldsymbol{\xi}}; L^q(\Re^3{}_{\mathbf{x}})) \tag{3.4.1}$$

and prove:

Theorem 3.4.1. *For any $s \in \Re$ and $q \in [1, 2]$, there is a constant $C \geq 0$ such that*

$$\| T(t)h \|_{H_s} \leq C(1+t)^{-m} \| h \|_{H_s \cap L^{q,2}}, \tag{3.4.2}$$

$$\| T(t)(I - P_0)h \|_{H_s} \leq C(1+t)^{-m-1/2} \| h \|_{H_s \cap L^{q,2}} \tag{3.4.3}$$

where $m = 3(2-q)/4q$.

Proof. By Parseval's equality for Fourier transforms we have

$$\| T(t)h \|_{H_s}^2 = \int (1 + |\mathbf{k}|^{2s}) \| T(t;\mathbf{k})\hat{h} \|_{L^2}^2 \, d\mathbf{k}. \tag{3.4.4}$$

Recalling Corollary 3.3.7, we split the integral into two contributions I_1 and I_2, referring to $|\mathbf{k}| \leq k_0$ and $|\mathbf{k}| \geq k_0$, respectively. Then I_2 is bounded by $\exp[-2(\nu_0 - \epsilon)t] \| h \|_{H_s}^2$ and

$$I_1 \leq C(\sum_{j=0}^{n+1} I_{j,1} + \exp[-2(\nu_0 - \epsilon)t] \| h \|_{H_s}^2) \tag{3.4.5}$$

where

$$I_{j,1} = \int_{|\mathbf{k}| \leq k_0} \exp(2\mathrm{Re}\mu_j(|\mathbf{k}|)t) \| \hat{h}(\mathbf{k}, .) \|_{L^2}^2 \,. \tag{3.4.6}$$

By Theorem 3.3.6, there is a positive constant σ, such that

$$\mathrm{Re}\mu_j(|\mathbf{k}|) \leq -\sigma|\mathbf{k}|^2 \qquad (j = 0, 1, \ldots, n+1, |\mathbf{k}| \leq k_0). \tag{3.4.7}$$

Then by Hölder's inequality,

$$I_{j,1} \leq \left[\int_{|\mathbf{k}| \leq k_0} \exp(-\sigma q' |\mathbf{k}|^2 t) d\mathbf{k} \right]^{1/q'} \| \hat{h}(\mathbf{k}, .) \|_{L^{2p'}(\Re_k^3; L_\xi^2(r^3))}^2 \tag{3.4.8}$$

where $(1/p' + 1/q' = 1)$. The integral is bounded by

$$\int_{|\mathbf{k}|\le k_0} \exp(-\sigma q'|\mathbf{k}|^2 t)d\mathbf{k} \le \exp[\sigma q' k_0^2] \int \exp[-\sigma q'|\mathbf{k}|^2(1+t)]d\mathbf{k} \le C(1+t)^{-3/2} \tag{3.4.9}$$

while the norm in (3.4.8), thanks to a well-known interpolation inequality for the Fourier transform[8], is bounded by

$$(2\pi)^{2-2/p'} \parallel\parallel h \parallel_{L^2}\parallel^2_{L^q} \le (2\pi)^{2-2/p'} \parallel\parallel h \parallel_{L^q}\parallel^2_{L^2} = (2\pi)^{2-2/p'} \parallel h \parallel^2_{L^{q,2}},$$

with $q = 2p'/(2p'-1)$, which proves (3.4.2). (Here we have used the fact, that, by convexity,

$$\parallel\parallel h \parallel_{L^2}\parallel_{L^q} \le \parallel\parallel h \parallel_{L^q}\parallel_{L^2},$$

for $q \le 2$.) To prove (3.4.3) we proceed in the same way, but now we take into account that we get an extra factor $|\mathbf{k}|^{q'}$ in the integral estimated in Eq. (3.4.9), thanks to Theorem 3.3.6; this leads to an exponent $3/2 + q'/2$ in place of $3/2$ and hence to an exponent $3/(2q') + 1/2$ in the final estimate (in place of the exponent $3/(2q')$). □

Remark 3.4.2. The exponent $m = 3(2-q)/4q$ in the previous theorem is larger than $1/2$ if $q \in [1, 6/5)$ and takes the maximum value $3/4$ for $q = 1$.

The result that we have just proved indicates that the solution decays in time and that the component orthogonal to the collision invariants decays just a little bit faster. Since we want to use this result as a tool for attacking the weakly nonlinear problem, we must face the problem that $\Gamma(h,h)$ is not well defined in H_s, but it is, as will be shown in the next section, in the space $H_{s,\beta}$ defined by:

$$h \in H_{s,\beta} \Rightarrow h \in L^\infty_{\text{loc}}(\Re^3_{\boldsymbol{\xi}}, H^s(\Re^3{}_{\mathbf{x}})),$$

$$\parallel h \parallel_{s,\beta} = \sup_{\boldsymbol{\xi}} (1+|\boldsymbol{\xi}|^2)^{\beta/2} \parallel h(\cdot,\boldsymbol{\xi}) \parallel_{H^s(R^3)} < \infty. \tag{3.4.10}$$

Hence, before proceeding further, we translate the decay estimates, which have just been found, into $H_{s,\beta}$, as first suggested by Grad[3]. Let us set

$$|h|_{m,s,\beta} = \sup_{t\ge 0}(1+t)^m \parallel h(t) \parallel_{s,\beta} \tag{3.4.11}$$

and prove the following

Theorem 3.4.3. *Let $q \in [1,2], s \in \Re, \beta \ge 0$ and $m = 3(2-q)/4q$ and $h = h(\mathbf{x},\boldsymbol{\xi})$ a function of $H_s \cap L^{q,2} \cap H_{s,\beta}$. Then there is a constant $C \ge 0$ such that, for any h,*

$$|T(t)(I-P_0)^n h|_{m+n/2,s,\beta} < C \parallel h \parallel_{H_s \cap L^{q,2} \cap H_{s,\beta}}\,. \tag{3.4.12}$$

Proof. This result can be obtained from the circumstance that the semigroup $U(t)$ generated by the operator $A = -\boldsymbol{\xi}\cdot\partial/\partial\mathbf{x} - \nu(\boldsymbol{\xi})I$ is related to the semigroup $T(t)$ generated by the full Boltzmann operator $B = A + K$, through

$$T(t)g = U(t)g + \int_0^t U(t-s)KT(s)gds. \tag{3.4.13}$$

Here g ("the initial data") is a function of $\mathbf{x}, \boldsymbol{\xi}$ belonging to some Banach space, such as those used before. Eq. (3.4.13) is nothing else than the integral form of Eq. (3.3.1), obtained by rewriting the latter as

$$\frac{\partial h}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial h}{\partial \mathbf{x}} + \nu(\boldsymbol{\xi})h = Kh \tag{3.4.14}$$

and integrating along the characteristic lines of the left-hand side. Let us put

$$|h|_{m,X} = \sup_{t\geq 0}(1+t)^m \parallel h(t) \parallel_X \tag{3.4.15}$$

a special case of which is Eq. (3.4.11). We are now going to exploit Theorem 3.2.4 and the fact that $\parallel U(t) \parallel \leq \exp(-\nu_0 t)$ in both H_s and $H_{s,\beta}$. Then Eq. (3.4.13) readily gives

$$|T(t)g|_{m,X} \leq C \parallel g \parallel_X + |T(t)g|_{m,Y} \tag{3.4.16}$$

for the pairs $X = H_{s,0}, Y = H_s$, and $X = H_{s,\beta+1}, Y = H_{s,\beta}, \beta \geq 0$. This permits an iterative use of this formula with respect to β to show that it holds for $X = H_{s,\beta}, Y = H_s$ $(\beta \geq 0)$ as well. The proof is now complete, because Theorem 3.4.1 gives an estimate of $\parallel T(t)g \parallel_{m,H_s}$. □

A problem we have to face when dealing with the nonlinear problem is that $\Gamma(h,h)$ is not bounded in $H_{s,\beta}$. In order to circumvent this difficulty, we shall need the smoothing properties of time integration, in the form of the following

Theorem 3.4.4. *Let us assume that* $0 \leq m' \neq 1/2, s \in \Re, \beta \geq 0$ *and* $0 \leq m < \min(2m', 5/4, 2m' + 1/4)$. *Then*

$$|Gh|_{m,s,\beta} < C(|h|_{2m',s,\beta} + |\nu h|_{2m',H_s\cap L^{1,2}}) \tag{3.4.17}$$

where

$$Gh = \int_0^t T(t-s)(I-P_0)\nu h(s)ds. \tag{3.4.18}$$

Proof. For any $\alpha \geq 0$ we have

$$|G_n h|_{m,s,\beta} \leq C|h|_{m,s,\beta} \qquad (n = 0, 1) \tag{3.4.19}$$

where

$$G_n h = \int_0^t U(t-s)(I-P_0)^n \nu h(s)ds \qquad (n = 0, 1). \tag{3.4.20}$$

In fact, taking the norm in $H^s(\Re^3_{\mathbf{x}})$, we have:

$$\begin{aligned}
\| G_n h \|_{H^s(\Re^3_{\mathbf{x}})} &\leq \int_0^t \exp[-\nu(\boldsymbol{\xi})(t-s)](I-P_0)^n \nu(\boldsymbol{\xi}) \| h(\cdot,\boldsymbol{\xi},s) \|_{H^s(\Re^3_{\mathbf{x}})} \, ds \\
&\leq C \int_0^t \exp[-\nu(\boldsymbol{\xi})(t-s)]\nu(\boldsymbol{\xi})(1+s)^{-m}(1+|\boldsymbol{\xi}|^2)^{-\beta/2}|h|_{m,s,\beta} ds \\
&\leq C(1+t)^{-m}|h|_{m,s,\beta}(1+|\boldsymbol{\xi}|^2)^{-\beta/2} \qquad (n=0,1)
\end{aligned} \tag{3.4.21}$$

where we have used the fact that $I - P_0$ is a bounded operator. Eq. (3.4.19) now easily follows. In order to obtain (3.4.17), we remark that

$$Gh = G_1 h + G_0([\nu(.)]^{-1} K G h) \tag{3.4.22}$$

and, proceeding as in the proof of (3.4.16), we obtain (for any $m \geq 0$)

$$|Gh|_{m,s,\beta} \leq C(|G_1 h|_{m,s,\beta} + |Gh|_{m,H^s}). \tag{3.4.23}$$

Combining this with Theorem 3.4.1 (for $q = 1$) yields (3.4.17). □

3.5 The Global Existence Theorem for the Nonlinear Equation

We now have all the preliminary results to be used to solve Eq. (3.1.3). Using the operator G defined in Eq. (3.4.18), we can write the corresponding integral equation in the following form:

$$h(t) = T(t)h_0 + G([\nu(.)]^{-1}\Gamma(h,h))(t) \equiv N(h)(t) \tag{3.5.1}$$

where Lemma 3.2.6 was taken into account. Eq. (3.5.1) shows that we must find a fixed point of the nonlinear mapping N. To this end, we first need

Lemma 3.5.1. *Let $m \geq 0, s > 3/2$ and $\beta > 2$. Then there is a constant $C \geq 0$ such that*

$$|[\nu(.)]^{-1}\Gamma(h,g)|_{2m,s,\beta} + |\Gamma(h,g)|_{2m,H_s \cap L^{1,2}} \leq C|h|_{m,s,\beta}|g|_{m,s,\beta}. \tag{3.5.2}$$

Proof. The theorem is a consequence of the following three facts: (i) $H_{s,\beta}$ is a Banach algebra, i.e., a Banach space closed with respect to multiplication) for $s > 3/2$; (ii) H_s is continuously imbedded in $H_{1,\beta}$ if $\beta > 3/2$; (iii) if $h, g \in L^2$, then $uv \in L^1$ (this is applied to the dependence upon $\mathbf{x}$). Consequently the lemma follows from Lemma 3.2.6. □

Let us take now $q \in [1,2]$ and set $m = m' = 3(2-q)/(4q)$ so that the conditions of Theorem 3.4.4 are satisfied. Combining Theorems 3.4.3 and 3.4.4 with Lemma 3.5.1, we see that the operator N appearing in Eq. (3.5.1) satisfies

$$|N(h)|_{m,s,\beta} \leq C_0 \| h_0 \|_{H_{s,\beta} \cap L^{q,2}} + C_1 |h|^2_{m,s,\beta},$$

$$|N(h) - N(g)|_{m,s,\beta} \leq C_1(|h|_{m,s,\beta} + |g|_{m,s,\beta})|h - g|_{m,s,\beta}. \tag{3.5.3}$$

This shows that N is contractive if h_0 is sufficiently small. We have thus proved

Theorem 3.5.2. *Let $q \in [1,2], s > 3/2$ and $\beta > 2$. Then there are positive constants c_0 and c_1, such that for any h_0 with*

$$\| h_0 \|_{H_{s,\beta}\cap L^{q,2}} \leq c_0 \tag{3.5.4}$$

Eq. (3.5.1) *has a unique global solution $h \in L^\infty([0,\infty); H_{s,\beta})$ satisfying*

$$|h|_{m,s,\beta} \leq c_1 \| h_0 \|_{H_{s,\beta}\cap L}\ q, 2 \qquad (m = 3(2-q)/(4q)). \tag{3.5.5}$$

This result was proved independently by N. B. Maslova and A. N. Firsov[5], Nishida and Imai[7] and Ukai[10], after the paper by Ukai[9] had given the basic results on the weakly nonlinear Boltzmann equation. In the latter paper Ukai had actually given a deeper result proving that the solution is more regular than proved in Theorem 3.5.2 and is actually a classical solution of the Boltzmann equation. In order to discuss this result, we define

$$\dot{H}_{s,\beta} = \{h \in H_{s,\beta}; \| [1 - \chi_R(|\boldsymbol{\xi}| + |\mathbf{k}|)]\hat{h} \|_{s,\beta} \to 0 \text{ as } R \to \infty\} \tag{3.5.6}$$

where $\mathbf{k}$ is the variable conjugate to $\mathbf{x}$ in the Fourier transform. Ukai and Asano[11] proved the following facts: (i) $U(t)$ and hence $T(t)$ are, for any s and β , C_0-semigroups on $\dot{H}_{s,\beta}$, although not in $H_{s,\beta}$, with the domains of the generators related by

$$D(A) = D(B) \supset \dot{H}_{s+1,\beta+1}. \tag{3.5.7}$$

Also

$$[\nu(.)]^{-1}\Gamma(.,.) \quad \text{maps} \quad \dot{H}_{s,\beta} \times \dot{H}_{s,\beta} \quad \text{into} \quad \dot{H}_{s,\beta} \quad \text{if} \quad s > 3/2, \beta \geq 0. \tag{3.5.8}$$

It follows that $N(h) \in C^0([0,\infty); \dot{H}_{s,\beta})$ if $h \in C^0([0,\infty); \dot{H}_{s,\beta})$ and if $h_0 \in \dot{H}_{s,\beta}$. Eq. (3.5.7) with $s-1, \beta-1$ in place of s, β leads then to

Theorem 3.5.3. *Let h, h_0 be as in Theorem* 3.5.2. *If, in addition, $h_0 \in \dot{H}_{s,\beta}$, then $h \in C^0([0,\infty); \dot{H}_{s,\beta}) \cap C^1([0,\infty); \dot{H}_{s-1,\beta-1})$ and is a classical solution of Eq.* (3.1.3) *with initial value h_0 and hence $f = M + M^{1/2}h$ is a classical solution of Eq.* (3.1.1).

Since $H_{s,\beta} \in \dot{H}_{s-\epsilon,\beta-\epsilon}$ for any $\epsilon > 0$, the above two theorems lead to the following

Theorem 3.5.4. *Let h, h_0 be as in Theorem* 3.5.2. *Then*

$$h \in L^\infty([0,\infty); H_{s,\beta}) \cap C^0([0,\infty); H_{s-\epsilon,\beta-\epsilon}) \cap C^1([0,\infty); H_{s-1-\epsilon,\beta-1-\epsilon})$$

($\epsilon > 0$) *and is a classical solution of Eq.* (3.1.3), *and hence $f = M + M^{1/2}h$ is a classical solution of Eq.* (3.1.1).

This is the theorem originally given by Ukai[9,10]; the conciseness of his papers as well as the fact that many readers did not appreciate the meaning of the "$-\epsilon$" in the subscripts of Theorem 3.5.4 generated the rumor, unfortunately echoed by some of the books on kinetic theory, that the statement of Ukai[9,10] was not completely correct, but this, as we have seen, is not the case.

3.6 Extensions: The Periodic Case and Problems in One and Two Dimensions

It is easy to see that the previous arguments also provide the global existence for the Cauchy problem for Eq. (3.1.3) when the solution is looked for in a box with periodicity boundary conditions. This result has a physical meaning because the solution of the problem in a box with specular reflection can be reduced[7] to that with periodicity conditions by considering 2^3 contiguous boxes, each of which is the mirror image of the neighboring ones.

In the periodic case, it is natural to use the Fourier series, instead of the Fourier integral. The proof is actually simpler because $\mathbf{k}$ is never close to the origin (unless $\mathbf{k} = 0$). Then Theorem 3.4.1 simplifies because the projection onto the subspace spanned by the collision invariants does not decay in time and the remaining part decays exponentially. We remark that the reason for the decay is different in the two cases. In a bounded domain, the dissipativity of L has a crucial role together with the fact that the natural basis for representing the space dependence of the solution is discrete (a Fourier series replaces the Fourier integral). In the case of $\Re^3$ the dispersion properties of the free-streaming operator ensure a decay (although not exponential) in time.

In fact Theorem 3.4.1 is now replaced by:

Theorem 3.6.1. *For any $s \in \Re$, there is a constant $\sigma_0 > 0$ such that*

$$\| T(t)h \|_{H_s} \leq C \| h \|_{H_s}, \tag{3.6.1}$$

$$\| T(t)(I - P_0)h \|_{H_s} \leq C \exp(-\sigma_0 t) \| h \|_{H_s} \tag{3.6.2}$$

where $C \geq 0$ is independent of u and $t \geq 0$.
Here, of course, $H_s = L^2(\Re^3{}_{\boldsymbol{\xi}}; H^s(T^3_{\mathbf{x}}))$, where $T^3_{\mathbf{x}}$ is a three-dimensional torus and (3.4.4) *is, e.g., replaced by*

$$\| T(t)h \|^2_{H_s} = \sum_{k \in Z^3} (1 + |\mathbf{k}|^{2s}) \| T(t;\mathbf{k})\hat{h}(\mathbf{k},.) \|^2_{L^2} . \tag{3.6.3}$$

Similarly, the other results for the case of $\Re^3$ can be translated into theorems for T^3 to arrive at the global existence result for the periodic case:

Theorem 3.6.2. *Let $s > 3/2$ and $\beta > 2$. Then there are positive constants c_0 and c_1, such that for any h_0 with*

$$\| h_0 \|_{H_{s,\beta}} \leq c_0, \tag{3.6.4}$$

Eq. (3.1.1) *associated with periodicity boundary conditions has a unique global solution* $h \in L^\infty([0,\infty); H_{s,\beta})$, *which, if, in addition,* $P_0 h_0 = 0$, *then* $P_0 u(t) = 0$ *for all* $t \geq 0$ *and*

$$\sup_{T\geq 0} \exp(\sigma_0 t)|h|_{m,s,\beta} \leq c_1. \tag{3.6.5}$$

For the sake of clarity, let us remark here that the projection P_0 is taken in the Hilbert space $L^2(\Re^3{}_{\boldsymbol{\xi}} \times T^3_{\mathbf{x}})$ and thus the restriction $P_0 h_0 = 0$ is not so important, because it can always be satisfied by an appropriate choice of the parameters in the Maxwellian M. This choice is, of course, not available in the case of $\Re^3{}_{\boldsymbol{\xi}} \times \Re^3{}_{\mathbf{x}}$, because the Maxwellian is constant in $\mathbf{x}$ and hence not integrable in $\Re^3{}_{\mathbf{x}}$.

Theorem 3.6.2 is due to S. Ukai[9] and was the first global existence theorem concerning the Cauchy problem for the space-inhomogeneous Boltzmann equation.

Another important remark concerns the solution of the Boltzmann equation when the data, and hence the solution, depend on just one or two space variables. The existence theorems in bounded domains apply without any difficulty, because one has only to restrict $\mathbf{k}$ to belong to Z and Z^2 rather than to Z^3. The matter is more delicate in one and two dimensions, because of the role played by the space dimension in the estimates of Theorem 3.6.1. As remarked by Ukai[12], however, the results remain valid in this case as well.

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Chapter 4

Boundary Value Problems

4.1 Boundary Conditions

The Boltzmann equation must be accompanied by boundary conditions, which describe the interaction of the gas molecules with solid or liquid walls. It is to this interaction that one can trace the origin of the drag and lift exerted by the gas on another body and the heat transfer between the gas and the boundaries.

The study of gas-surface interaction may be regarded as a bridge between the kinetic theory of gases and solid state physics and is an area of research by itself. The difficulties of a theoretical investigation are due, mainly, to our lack of knowledge of the structure of surface layers of solid and liquid bodies and hence of the effective interaction potential of the gas molecules with the wall. When a molecule impinges upon a surface, it is adsorbed and may form chemical bonds, dissociate, become ionized or displace surface molecules. Its interaction with the solid surface depends on the surface finish, the cleanliness of the surface, its temperature, etc. It may also vary with time because of outgassing from the surface. Preliminary heating of a surface also promotes purification of the surface through emission of adsorbed molecules. In general, adsorbed layers may be present; in this case, the interaction of a given molecule with the surface may also depend on the distribution of molecules impinging on a surface element. For a more detailed discussion the reader should consult Refs. 15 and 31.

In general, a molecule striking a surface with a velocity $\boldsymbol{\xi}'$ reemerges from it with a velocity $\boldsymbol{\xi}$ which is strictly determined only if the path of the molecule within the wall can be computed exactly. This computation is very hard, because it depends upon a great number of details, such as the locations and velocities of all the molecules of the wall and an accurate knowledge of the interaction potential. Hence it is more convenient to think in terms of a probability density $R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau)$ that a molecule striking the surface with velocity between $\boldsymbol{\xi}'$ and $\boldsymbol{\xi}' + d\boldsymbol{\xi}'$ at the point $\mathbf{x}$ and time t will re-emerge at practically the same point with

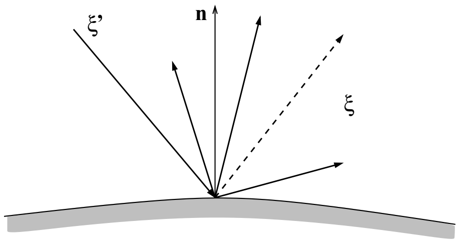

Figure 4.1: The velocity $\boldsymbol{\xi}$ of a re-emerging molecule is not uniquely determined by the velocity possessed by the same molecule before hitting the wall, unless specular reflection applies (dashed line).

a velocity between $\boldsymbol{\xi}$ and $\boldsymbol{\xi} + d\boldsymbol{\xi}$ (Fig. 4.1) after a time interval τ (adsorption or sitting time). If the function (or distribution) R is known, then we can easily write down the boundary condition for the distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$. To simplify the discussion, the surface will be assumed to be at rest.

The mass of the molecules emerging with a velocity between $\boldsymbol{\xi}$ and $\boldsymbol{\xi} + d\boldsymbol{\xi}$ from a surface element dA about $\mathbf{x}$ in the time interval between t and $t + dt$ is

$$d^*\mathcal{M} = f(\mathbf{x}, \boldsymbol{\xi}, t)|\boldsymbol{\xi} \cdot \mathbf{n}| dt dA d\boldsymbol{\xi} \qquad (\mathbf{x} \in \partial\Omega, \boldsymbol{\xi} \cdot \mathbf{n} > 0) \tag{4.1.1}$$

where $\mathbf{n}$ is the unit vector normal to the surface $\partial\Omega$ at $\mathbf{x}$ and directed from the wall into the gas. Analogously, the probability that a molecule impinges upon the same surface element with velocity between $\boldsymbol{\xi}'$ and $\boldsymbol{\xi}' + d\boldsymbol{\xi}'$ in the time interval between $t - \tau$ and $t - \tau + dt$ ($\tau > 0$) is

$$d^*\mathcal{M}' = f(\mathbf{x}, \boldsymbol{\xi}', t - \tau)|\boldsymbol{\xi}' \cdot \mathbf{n}| dt dA d\boldsymbol{\xi}' \qquad (\mathbf{x} \in \partial\Omega, \boldsymbol{\xi}' \cdot \mathbf{n} < 0). \tag{4.1.2}$$

If we multiply $d^*\mathcal{M}'$ by the probability of a scattering event from velocity $\boldsymbol{\xi}'$ to a velocity between $\boldsymbol{\xi}$ and $\boldsymbol{\xi} + d\boldsymbol{\xi}$ with an adsorption time between τ and $\tau + d\tau$ (i.e., $R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) d\boldsymbol{\xi} d\tau$) and integrate over all the possible values of $\boldsymbol{\xi}'$ and τ, we must obtain $d^*\mathcal{M}$ (here we assume that each molecule re-emerges from the surface element into which it entered, which is not so realistic when τ is large):

$$d^*\mathcal{M} = d\boldsymbol{\xi} \int_0^\infty d\tau \int_{\boldsymbol{\xi}' \cdot \mathbf{n} < 0} R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) d^*\mathcal{M}' \qquad (\mathbf{x} \in \partial\Omega, \boldsymbol{\xi} \cdot \mathbf{n} > 0). \tag{4.1.3}$$

Equating the expressions in Eqs. (4.1.1) and (4.1.3) and cancelling the common factor $dAd\boldsymbol{\xi}dt$, we obtain

$$f(\mathbf{x}, \boldsymbol{\xi}, t)|\boldsymbol{\xi} \cdot \mathbf{n}| = \int_0^\infty d\tau \int_{\boldsymbol{\xi}' \cdot \mathbf{n} < 0} R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) f(\mathbf{x}, \boldsymbol{\xi}', t - \tau)|\boldsymbol{\xi}' \cdot \mathbf{n}| d\boldsymbol{\xi}'$$
$$(\mathbf{x} \in \partial\Omega, \boldsymbol{\xi} \cdot \mathbf{n} > 0). \tag{4.1.4}$$

The kernel R can be assumed to be independent of f under suitable conditions which we shall not detail here[15,31]. If, in addition, the effective adsorption time is small compared to any characteristic time of interest in the evolution of f, we can let $\tau = 0$ in the argument of f appearing in the right-hand side of Eq. (4.2.4); in this case the latter becomes:

$$f(\mathbf{x}, \boldsymbol{\xi}, t)|\boldsymbol{\xi} \cdot \mathbf{n}| = \int_{\boldsymbol{\xi}' \cdot \mathbf{n} < 0} R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) f(\mathbf{x}, \boldsymbol{\xi}', t)|\boldsymbol{\xi}' \cdot \mathbf{n}| d\boldsymbol{\xi}' \quad (\mathbf{x} \in \Omega, \boldsymbol{\xi} \cdot \mathbf{n} > 0) \tag{4.1.5}$$

where

$$R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) = \int_0^\infty d\tau R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau). \tag{4.1.6}$$

Eq. (4.1.5) is, in particular, valid for steady flow problems.

Although the idea of a scattering kernel had appeared before, it is only at the end of the 1960s that a systematic study of the properties of this kernel appears in the scientific literature[16,17,22,23]. In particular, the following properties were pointed out[15–18,23,31–32]:

1) *Nonnegativity*, i.e., R cannot take negative values:

$$R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) \geq 0 \tag{4.1.7}$$

and, as a consequence

$$R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) \geq 0. \tag{4.1.8}$$

2) *Normalization*, if permanent adsorption is excluded; i.e., R, as a probability density for the totality of events, must integrate to unity:

$$\int_0^\infty d\tau \int_{\boldsymbol{\xi}' \cdot \mathbf{n} \geq 0} R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) d\boldsymbol{\xi} = 1 \tag{4.1.9}$$

and, as a consequence

$$\int_{\boldsymbol{\xi}' \cdot \mathbf{n} \geq 0} R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) d\boldsymbol{\xi} = 1. \tag{4.1.10}$$

3) *Reciprocity*; this is a subtler property that follows from the circumstance that the microscopic dynamics is time reversible and the wall is assumed to be in a local equilibrium state, not significantly disturbed by the impinging molecule. It reads as follows:

$$|\boldsymbol{\xi}' \cdot \mathbf{n}| M_w(\boldsymbol{\xi}') R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t; \tau) = |\boldsymbol{\xi} \cdot \mathbf{n}| M_w(\boldsymbol{\xi}) R(-\boldsymbol{\xi} \to -\boldsymbol{\xi}'; \mathbf{x}, t; \tau) \tag{4.1.11}$$

and, as a consequence

$$|\boldsymbol{\xi}' \cdot \mathbf{n}| M_w(\boldsymbol{\xi}') R(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) = |\boldsymbol{\xi} \cdot \mathbf{n}| M_w(\boldsymbol{\xi}) R(-\boldsymbol{\xi} \to -\boldsymbol{\xi}'; \mathbf{x}, t)\,. \tag{4.1.12}$$

Here M_w is a (nondrifting) Maxwellian distribution having the temperature of the wall, which is uniquely identified apart from a factor.

We remark that the reciprocity and the normalization relations imply another property:

3$'$) *Preservation of equilibrium*, i.e., the Maxwellian M_w must satisfy the boundary condition (4.1.4):

$$M_w(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\mathbf{n}| = \int_0^\infty d\tau \int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0} R(\boldsymbol{\xi}'\to\boldsymbol{\xi};\mathbf{x},t;\tau)M_w(\boldsymbol{\xi}')|\boldsymbol{\xi}'\cdot\mathbf{n}|d\boldsymbol{\xi}' \tag{4.1.13}$$

equivalent to

$$M_w(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\mathbf{n}| = \int_{\boldsymbol{\xi}'\cdot\mathbf{n}<0} R(\boldsymbol{\xi}'\to\boldsymbol{\xi};\mathbf{x},t)M_w(\boldsymbol{\xi}')|\boldsymbol{\xi}'\cdot\mathbf{n}|d\boldsymbol{\xi}'. \tag{4.1.14}$$

In order to obtain Eq. (4.1.13) it is sufficient to integrate Eq. (4.1.11) with respect to $\boldsymbol{\xi}'$ and τ, taking into account Eq. (4.1.9) (with $-\boldsymbol{\xi}$ and $-\boldsymbol{\xi}'$ in place of $\boldsymbol{\xi}'$ and $\boldsymbol{\xi}$, respectively. We remark that one frequently assumes Eq. (4.1.13) (or (4.1.14)), without mentioning Eq. (4.1.11) (or (4.1.12)); although this is enough for many purposes, reciprocity is very important when constructing mathematical models, because it places a strong restriction on the possible choices.

The scattering kernel is a fundamental concept in gas-surface interaction, by means of which other quantities should be defined. Frequently its use is avoided by using the so-called accommodation coefficients, with the consequence of lack of clarity, misinterpretation of experiments, bad definitions of terms and misunderstanding of concepts. The basic information on gas-surface interaction, which should be in principle obtained from a detailed calculation based on a physical model, is summarized in a scattering kernel. The further reduction to a small set of accommodation coefficients can be advocated for practical purposes, provided this concept is firmly related to the scattering kernel.

In order to describe the accommodation coefficients in a systematic way, it is convenient to introduce, for any pair of functions ϕ and ψ, the notations

$$(\psi,\phi)_+ = \int_{\boldsymbol{\xi}\cdot\mathbf{n}>0} \psi(\boldsymbol{\xi})\phi(\boldsymbol{\xi})M_w(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\mathbf{n}|d\boldsymbol{\xi}, \tag{4.1.15}$$

$$(\psi,\phi)_- = \int_{\boldsymbol{\xi}\cdot\mathbf{n}<0} \psi(\boldsymbol{\xi})\phi(\boldsymbol{\xi})M_w(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\mathbf{n}|d\boldsymbol{\xi}. \tag{4.1.16}$$

Now, if we factor M_w out of the distribution function f and write

$$f = M_w\phi, \tag{4.1.17}$$

we can define the accommodation coefficient for the quantity ψ when the distribution function at the wall is $M_w\phi$, in the following way:

$$\alpha(\psi,\phi) = [(\psi,\phi)_- - (\psi,\phi)_+]/[(\psi,\phi)_- - (\psi,\iota)_+] \tag{4.1.18}$$

where ι denotes a constant function, such that

$$(\iota, \iota)_+ = (\iota, \phi)_+. \tag{4.1.19}$$

Physically the numerator in Eq. (4.1.18) is the difference between the impinging and emerging flow of the quantity, whose density is ψ, when the distribution is $M_w\phi$; the denominator is the same thing when the restriction of f to $\boldsymbol{\xi}\cdot\mathbf{n} > 0$ is replaced by the wall Maxwellian, normalized in such a way as to give the same entering flow rate as f. In particular, if we let $\psi = \boldsymbol{\xi}\cdot\mathbf{n}$, we obtain the accommodation coefficient for normal momentum; if we let $\psi = \boldsymbol{\xi}\cdot\mathbf{t}$, we obtain the accommodation coefficient for tangential momentum (in the direction of the unit vector $\mathbf{t}$, tangent to the wall); if we let $\psi = |\boldsymbol{\xi}|^2$, we obtain the energy accommodation coefficient. It is convenient to restrict the definition in Eq. (4.1.18) to functions enjoying the property $\psi(\boldsymbol{\xi}) = \psi(\boldsymbol{\xi} - 2\mathbf{n}(\mathbf{n}\cdot\boldsymbol{\xi}))$, which are even functions of $\boldsymbol{\xi}\cdot\mathbf{n}$. This condition is not satisfied by $\psi = \boldsymbol{\xi}\cdot\mathbf{n}$; accordingly, if one wants to define an accommodation coefficient for normal momentum, he has to take $\psi = |\boldsymbol{\xi}\cdot\mathbf{n}|$.

In general, $\alpha(\psi, \phi)$ turns out to depend upon the distribution function of the impinging molecule; accordingly the definition (4.1.18) is not so useful, in general. It becomes more useful if one selects[15,31] a particular class of functions ϕ.

It is clear that there is a relation between the accommodation coefficients and the scattering kernel $R(\boldsymbol{\xi}' \to \boldsymbol{\xi})$ (we omit indicating the space and time arguments), but what this particular relation is depends on the set of functions from which ϕ and ψ are chosen[15,31].

In view of the difficulty of computing the kernel $R(\boldsymbol{\xi}' \to \boldsymbol{\xi})$ from a physical model of the wall, a different procedure, which is less physical in nature, is usually adopted. The idea is to construct a mathematical model in the form of a kernel $R(\boldsymbol{\xi}' \to \boldsymbol{\xi})$ which satisfies the basic physical requirements expressed by Eqs. (4.1.8), (4.1.10), (4.1.12) and is not otherwise restricted except by the condition of not being too complicated.

One of the simplest kernels is

$$R(\boldsymbol{\xi}' \to \boldsymbol{\xi}) = \alpha M_w(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\mathbf{n}| + (1-\alpha)\delta(\boldsymbol{\xi} - \boldsymbol{\xi}' + 2\mathbf{n}(\boldsymbol{\xi}'\cdot\boldsymbol{\xi})) \qquad (0 \le \alpha \le 1). \tag{4.1.20}$$

This kernel corresponds to Maxwell's model[36], according to which a fraction $(1-\alpha)$ of molecules undergoes a specular reflection, while the remaining fraction α is diffused with the Maxwellian distribution of the wall M_w. This is the only model for the scattering kernel that appeared in the literature before the late 1960s. Another model is the so-called Cercignani–Lampis (CL) model[23], which reads as follows:

$$\begin{aligned} &R(\boldsymbol{\xi}' \to \boldsymbol{\xi}) \\ &= \frac{[\alpha_n\alpha_t(2-\alpha_t)]}{\pi/2}\beta_w^2\boldsymbol{\xi}_n \exp\left[-\beta_w\frac{\boldsymbol{\xi}_n^2 + (1-\alpha_n)\boldsymbol{\xi}_n'^2}{\alpha_n} - \beta_w\frac{|\boldsymbol{\xi}_t - (1-\alpha_t)\boldsymbol{\xi}_t'|^2}{\alpha_t(2-\alpha_t)}\right] \\ &\quad \times I_0\left(\beta_w\frac{(1-\alpha_n)^{1/2}\boldsymbol{\xi}_n\boldsymbol{\xi}_n'}{\alpha_n}\right) \end{aligned} \tag{4.1.21}$$

where I_0 denotes the modified Bessel function of first kind and zeroth order defined by

$$I_0(y) = (2\pi)^{-1} \int_0^{2\pi} \exp(y \cos\phi) d\phi. \tag{4.1.22}$$

The two parameters α_t and α_n have a simple meaning; the first one is the accommodation coefficient for the tangential components of momentum, the second one the accommodation coefficient for $\boldsymbol{\xi}_n^2$, hence for the part of kinetic energy associated with the normal motion.

These models discussed above contain pure diffusion according to a non-drifting Maxwellian as a limiting case (Eq. (4.1.20) with $\alpha = 1$). The use of this particular model is justified for low-velocity flows over technical surfaces, but is inaccurate for flows with orbital velocity.

It is remarkable that, for any scattering kernel satisfying the three properties of normalization, positivity and preservation of equilibrium, a simple inequality holds. The latter was stated by Darrozès and Guiraud[24] who also sketched a proof. More details were given later[18,15]. The inequality follows from a convexity argument and reads as follows:

$$\mathcal{J}_n = \int_{R^3} \boldsymbol{\xi} \cdot \mathbf{n} f \log f d\boldsymbol{\xi} \leq -(2RT_w)^{-1} \int_{R^3} \boldsymbol{\xi} \cdot \mathbf{n} |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi} \qquad (\mathbf{x} \in \partial\Omega)\,. \tag{4.1.23}$$

Equality holds if and only if f coincides with M_w (the wall Maxwellian) on $\partial\Omega$ (unless the kernel in Eq. (4.1.5) is a delta function). We remark that if the gas does not slip upon the wall, the right-hand side of Eq. (4.1.23) equals $-q_n/(RT_w)$ where q_n is the heat flow along the normal, according to its definition given in Section 5. If the gas slips on the wall, then one must add the power of the stresses $\mathbf{p}_n \cdot \mathbf{v}$ to q_n. In any case, however, the right-hand side equals $q_n^{(w)}$, where $q_n^{(w)}$ is the heat flow in the solid at the interface, because the normal energy flow must be continuous through the wall and stresses have vanishing power in the solid, because the latter is at rest. If we identify the function H introduced in Section 1.7 with $-\eta/R$ (where η is the entropy of the gas), the inequality in Eq. (4.1.23) is exactly what one would expect from the Second Principle of thermodynamics.

4.2 Initial-Boundary and Boundary Value Problems

The global existence of a weak solution for the Cauchy problem for the Boltzmann equation, first obtained by DiPerna and Lions[26], was presented in Chapter 2. The proof applies to nonnegative data with finite energy and entropy. In this chapter, we shall first deal with the initial boundary value problem which arises when we consider the time evolution of a rarefied gas in a vessel Ω whose boundaries are kept at constant temperature. We shall assume that Ω is a bounded open set of $\Re^3$ with a sufficiently smooth boundary $\partial\Omega$. On $\partial\Omega$ we impose a linear boundary condition of the form envisaged in the previous section, when the molecules are assumed to be re-emitted by the surface with negligible delay. This boundary condition is given by Eq. (4.1.5) with a kernel enjoying the properties expressed by Eqs. (4.1.8), (4.1.10) and (4.1.14). We rewrite these equations below in a form appropriate for the study of a boundary value problem. $\mathbf{n} = \mathbf{n}(\mathbf{x})$ will always denote the inner normal at $\mathbf{x} \in \partial\Omega$.

$$\gamma_D^+ f(t, \mathbf{x}, \boldsymbol{\xi}) = \int_{\boldsymbol{\xi}' \cdot \mathbf{n} < 0} K(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) \gamma_D^- f(t, \mathbf{x}, \boldsymbol{\xi}') d\boldsymbol{\xi}' \equiv K \gamma_D^- f \tag{4.2.1}$$

$(\mathbf{x} \in \partial\Omega, \quad \boldsymbol{\xi} \cdot \mathbf{n} > 0)$,

$$K(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) \geq 0, \tag{4.2.2}$$

$$\int_{\boldsymbol{\xi} \cdot \mathbf{n} > 0} K(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) |\boldsymbol{\xi} \cdot \mathbf{n}| d\boldsymbol{\xi} = |\boldsymbol{\xi}' \cdot \mathbf{n}|, \tag{4.2.3}$$

$$M_w(\boldsymbol{\xi}) = \int_{\boldsymbol{\xi}' \cdot \mathbf{n} < 0} K(\boldsymbol{\xi}' \to \boldsymbol{\xi}; \mathbf{x}, t) M_w(\boldsymbol{\xi}') d\boldsymbol{\xi}', \tag{4.2.4}$$

where M_w is the wall Maxwellian and $\gamma_D^\pm$ are the so-called trace operators on $E^\pm = \{(t, \mathbf{x}, \boldsymbol{\xi}) \in \partial\Omega \times \Re^3 \times [0, T] \mid \pm \boldsymbol{\xi} \cdot \mathbf{n}(\mathbf{x}) > 0\}$. These operators permit one to define "the values taken on the boundary" $\gamma_D^\pm f$ (a.e. in $\boldsymbol{\xi} \in \Re^3$ and $x \in \partial\Omega$) by a function f for which this concept is not *a priori* defined (such as a function $f \in L^1(\Omega \times \Re^3)$). Of course one must show that these operators are well defined. Actually this is one of the main points in the extension of the proof of the DiPerna and Lions Theorem to the case under consideration.

The first existence theorem that we shall deal with was proved by Hamdache[29] in the case when the trace $\gamma_D^+ f$ is a linear combination (with weights summing up to unity) of the right-hand side of Eq. (4.1.1) and a given function. Here, we shall restrict ourselves to the case when the weight of the second term is zero because, as remarked by Hamdache[29], the real problems arise in this case.

Hamdache's result is important not only for its own sake, but also because it leads to discussing the long time behavior of the solution and its trend to a Maxwellian distribution when $t \to \infty$, a problem which has been hotly debated for many years, since Boltzmann first established his H-theorem. In Section 5 we shall discuss in detail the results of Desvillettes[25] and Cercignani[19] who have shown that the solution can be proved to tend asymptotically to a Maxwellian (in a weak sense).

More difficult cases refer to a boundary along which the temperature is not constant, or moving boundaries. The case of a non-isothermal boundary has been treated by Arkeryd and Cercignani[3], but only with a cutoff for large velocities, and we shall not discuss it here. Another topic which should be treated in this chapter is the pure boundary value problem which arises when we look for the asymptotic state of general initial-boundary value problems. The results on these problems, however, are scanty. Thus we shall restrict ourselves to the particular case of solutions close to equilibrium, while the general case will be the subject of a few remarks at the end of the chapter.

One of the key points in the proofs will be the inequality (4.1.26) which we state here as

Lemma 4.2.1. *If Eqs.* (4.2.1), (4.2.2), (4.2.3) *and* (4.2.4) *hold, then*

$$\int \boldsymbol{\xi}\cdot\mathbf{n}\gamma_D f\log\gamma_D f d\boldsymbol{\xi} \leq -\beta_w \int \boldsymbol{\xi}\cdot\mathbf{n}|\boldsymbol{\xi}|^2\gamma_D f d\boldsymbol{\xi} \tag{4.2.5}$$

(a.e. in t and $x \in \partial\Omega$) where β_w is the inverse temperature at a point $x \in \partial\Omega$. Unless the kernel in Eq. (4.1.1) *is a delta function, equality holds if and only if the trace $\gamma_D f$ of f on $\partial\Omega$ coincides with M_w (the wall Maxwellian).*

The trace operator γ_D has been informally defined in the lines following (4.2.4). Before stating Hamdache's theorem (in a slightly more general form) we have to report some trace results giving the L^1 regularity of the trace of f on the boundary and to study the semigroup generated by the free streaming operator.

There are general results of Ukai[38] on the traces of the solutions. To describe them we first define

$$\Lambda f = \frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\frac{\partial f}{\partial x} \tag{4.2.6}$$

and assume that $\partial\Omega$ is piecewise C^1.

We denote by $S^t(\mathbf{x},\boldsymbol{\xi})$ the pair $(\mathbf{x}+\boldsymbol{\xi}t,\boldsymbol{\xi})$ which gives the position and velocity of a molecule initially located at $(\mathbf{x},\boldsymbol{\xi})$ as long as $\mathbf{x}+\boldsymbol{\xi}t$ stays in Ω. Denote the forward ($t>0$) stay time in Ω by $t^+(\mathbf{x},\boldsymbol{\xi})$ and the backward one by $t^-(\mathbf{x},\boldsymbol{\xi})$. Then $S^t(\mathbf{x},\boldsymbol{\xi}) \in \Omega\times\Re^3$ for $-t^-(\mathbf{x},\boldsymbol{\xi}) < t < t^+(\mathbf{x},\boldsymbol{\xi})$ and $S^t(\mathbf{x},\boldsymbol{\xi}) \in \partial\Omega\times\Re^3$ for $t = t^\pm(\mathbf{x},\boldsymbol{\xi})$ if $t^\pm(\mathbf{x},\boldsymbol{\xi}) < \infty$. Let us also define $\Sigma^\pm = \{(\mathbf{x},\boldsymbol{\xi}) \in \partial\Omega\times\Re^3 \mid \pm\boldsymbol{\xi}\cdot\mathbf{n}(\mathbf{x}) > 0\}$ and remark that $S^t(\mathbf{x},\boldsymbol{\xi})$ exists for $(\mathbf{x},\boldsymbol{\xi}) \in \Sigma^\mp$ with $t^\pm = 0, t^\mp > 0$. In any case $S^t \in \overline{\Sigma^\mp}$ at $t = \pm t^\pm$. It is now convenient to write $r = (t,\mathbf{x},\boldsymbol{\xi})$ and for $T > 0$ define

$$\begin{aligned} &D = (0,T)\times\Omega\times\Re^3; \quad V^\pm = \{T^\pm\}\times\Omega\times\Re^3 \qquad (\text{where } T^+ = 0,\ T^- = T), \\ &E^\pm = (0,T)\times\Sigma^\pm; \quad \partial D^\pm = E^\pm \cup V^\pm \qquad (\text{same sign throughout}). \end{aligned} \tag{4.2.7}$$

The world line of a molecule passing through $r = (t,\mathbf{x},\boldsymbol{\xi}) \in D\cup\partial D^+\cup\partial D^-$ is given by

$$R^s(r) = (t+s,\mathbf{x}+\boldsymbol{\xi}s,\boldsymbol{\xi}) \qquad -s^-(r) \leq s \leq s^+(r) \tag{4.2.8}$$

where $s^\pm(r) = \min(T^\mp \mp t, t^\pm(\mathbf{x},\boldsymbol{\xi}))$ and $T^\mp$ are defined as in Eq. (4.2.7). Obviously

$$R^s(r) \in D \qquad (-s^-(r) < s < s^+(r)), R^s(r) \in \overline{\partial D^\mp} \qquad (s = s^\pm(r)). \tag{4.2.9}$$

Clearly if $f \in L^1(D)$, then $f(R^s(r))$ as a function of s is in $L^1(-s^-(r), s^+(r))$ for almost all $r \in \partial D^\pm$ and

$$\int_D f(r)dr = \int_{\partial D^\pm}\int_{s^-(r)}^{s^+(r)} f(R^s(r))dsd\sigma^\pm \tag{4.2.10}$$

holds, where

$$dr = dtd\mathbf{x}d\boldsymbol{\xi}; d\sigma^{\pm} = |\mathbf{n}(\mathbf{x}) \cdot \boldsymbol{\xi}|dtd\sigma d\boldsymbol{\xi} \quad (\text{on } E^{\pm}); \quad d\sigma^{\pm} = d\mathbf{x}d\boldsymbol{\xi} \quad (\text{on } V^{\pm}), \tag{4.2.11}$$

$\mathbf{n}(\mathbf{x})$ being the inward normal to $\partial\Omega$ and $d\sigma$ the usual measure on $\partial\Omega$. We set

$$(f, g) = \int_D f\overline{g}dr,$$

$$< \phi, \psi >_{\pm} = < \phi, \psi >_{E^{\pm}} + < \phi, \psi >_{V^{\pm}} = \int_{\partial D^{\pm}} \phi\overline{\psi}d\sigma^{\pm} \tag{4.2.12}$$

where, of course,

$$< \phi, \psi >_{E^{\pm}} = \int_{E^{\pm}} \phi\overline{\psi}|\mathbf{n}(\mathbf{x}) \cdot \boldsymbol{\xi}|dtd\sigma d\boldsymbol{\xi}, < \phi, \psi >_{V^{\pm}} = \int_{\mathbf{v}} \phi\overline{\psi}d\mathbf{x}d\boldsymbol{\xi} \quad (\text{for } t = T^{\pm}). \tag{4.2.13}$$

The trace theorem due to Ukai[38] holds between the spaces

$$W^p = \{f \in L^p(D) | \Lambda f \in L^p(D)\}, \qquad L_\theta^{p,\pm} = L^p(\partial D^{\pm}; \theta d\sigma^{\pm}),$$

$$\theta = \theta(r) = \min(1, s^+(r) + s^-(r)) \tag{4.2.14}$$

where Λf is defined in the distribution sense.

The trace operators $\gamma_D^{\pm}$ are first defined on $C_0^1(\overline{D})$ by

$$\gamma_D^{\pm} f = f|_{\partial D^{\pm}}, \qquad f \in C_0^1(\overline{D}). \tag{4.2.15}$$

Ukai[38] proved the following

Theorem 4.2.1. *Let $p \in [1, \infty]$, $\gamma_D^{\pm}$ have extensions in $\mathbf{B}(W^p, L_\theta^{p,\pm})$, the space of bounded linear operators from W^p to $L_\theta^{p,\pm}$. We denote these extensions again by $\gamma_D^{\pm}$. Thus it holds that*

$$\| \gamma_D^{\pm} f \|_{L_\theta^{p,\pm}} \leq C \| f \|_{W^p} = C(\| f \|_{L^p(D)} + \| \Lambda f \|_{L^p(D)}). \tag{4.2.16}$$

For the proof, see Refs. 38 and 22.

We cannot remove the weight function θ if $p < \infty$ in Eq. (4.2.16). For this reason, some authors[12,44] have obtained just $L_{\text{loc}}^{p,\pm}$ -traces. In order to solve the initial-boundary value problem, however, the $L_\theta^{p,\pm}$-traces are not adequate. We need $L^{p,\pm}$ traces defined by

$$L^{p,\pm} = L^p(\partial D^{\pm}; d\sigma^{\pm}) \tag{4.2.17}$$

We remark that $L^{p,\pm} = L_\theta^{p,\pm}$ for $p = \infty$ but $L^{p,\pm} \subseteq L_\theta^{p,\pm}$ if $p < \infty$. Let us also define, for future use,

$$\hat{W}^p = \{f \in W^p(D) | \ \gamma_D^{\pm} f \in L^{p,\pm}\} \subset W^p. \tag{4.2.18}$$

If we impose suitable boundary conditions, then we can make some progress in the direction of proving that $f \in \hat{W}^p$. To this end it is expedient to follow Ukai[38], who proved the following

Theorem 4.2.2. *Let $f \in W^p$, $p \in [1, \infty)$. If $\gamma_D^{\pm} f \in L^{p,\pm}$ (only one sign throughout), then $\gamma_D^{\mp} f \in L^{p,\mp}$. In this case, the following relation holds:*

$$\| \gamma_D^- f(r) \|_{L^{p,-}}^p = \| \gamma_D^+ f(r) \|_{L^{p,+}}^p + p\mathrm{Re} \int_D |f|^{p-2} \overline{f} \Lambda f dr \tag{4.2.19}$$

where "Re" denotes the real part.

For the proof, see Refs. 38 and 22.

This theorem immediately allows us to deduce the existence of the traces when f is assigned on ∂D^+, as a function of $L^{p,+}$. The situation is more complicated, if the boundary conditions are less trivial. We shall assume that boundary conditions of the form (4.1.1) are satisfied and prove the existence of the traces on the boundary, under suitable assumptions.

There is an important comment to be made on the case $p = 1$. One might doubt, in fact, the results which have been just discussed, because a smooth sequence of functions with bounded $L^{1,-}$ norm might tend to a measure. It is easy, however, to check that the trace exists locally around any $r = (\mathbf{x}, \boldsymbol{\xi}, t) \in \partial\Omega \times \Re^3 \times \Re_+$ with $\boldsymbol{\xi} \cdot \mathbf{n}(\mathbf{x}) \neq 0$. In fact one can prove[38,22]that

$$\hat{f}(s, r) = \hat{f}(s', r) + \int_{s'}^{s} \widehat{(\Lambda f)}(\tau, r) d\tau. \tag{4.2.20}$$

If we apply this relation to ϕf, where $f \in C_0^\infty(\Omega \times \Re^3 \times \Re_+)$ with $\phi = 1$ in a neighborhood of r on the boundary and with sufficiently small support not to involve any outgoing point if r is ingoing and conversely, we obtain, e.g.,

$$\widehat{\phi f}(s_+(r), r) = \int_{s_- r}^{s_+(r)} \widehat{\Lambda(\phi f)}(\tau, r) d\tau. \tag{4.2.21}$$

This is sufficient to prove that $\gamma_D f$ is locally in L^1 outside of $\boldsymbol{\xi} \cdot \mathbf{n}(\mathbf{x}) = 0$; the latter set is killed, however, in the $L^{1,\pm}$ norms.

In order to simplify the formal aspects of the treatment, we suppress the time derivative from Λ, and correspondingly the parts of the boundaries $\partial D^{\pm}$ corresponding to $t = 0$ and $t = T$ and integrations with respect to t; in fact these details do not play any role in what follows. Let us remark that when Eq. (4.1.1) holds, we easily obtain for $\phi \in W^\infty(D)$ and $f \in W^1(D)$:

$$< \gamma_D^- \phi(r), \gamma_D^- f(r) >_- = < \gamma_D^+ \phi(r), K\gamma_D^- f(r) >_+ + \int_D \phi(\Lambda f) dr + \int_D f(\Lambda \phi) dr. \tag{4.2.22}$$

If we take the value of ϕ on the boundary to be L^∞ and (distributionally) $\Lambda\phi = 0$, Eq. (4.2.12) shows that

$$\| \gamma_D^{\pm} \phi \|_{L^{\infty,\pm}} = \| \phi \|_{L^\infty(D)} \tag{4.2.23}$$

and in Eq. (4.2.22) the last term disappears.

We can now introduce the operator P which reflects $\boldsymbol{\xi}$, defined by $(Pf(\boldsymbol{\xi}) = f(-\boldsymbol{\xi}))$, and rewrite (4.2.22) as follows:

$$< \gamma_D^- \phi(r) - (PK)^\dagger P \gamma_D^+ \phi(r), \gamma_D^- f(r) >_- = \int_D \phi(\Lambda f) dr \quad (\Lambda\phi = 0) \qquad (4.2.24)$$

where $(PK)^\dagger$ is the dual operator of PK with respect to $< \cdot, \cdot >_-$. Let us put

$$\psi = \gamma_D^- \phi(r) - (PK)^\dagger P \gamma_D^+ \phi(r). \qquad (4.2.25)$$

We remark that if we take $\gamma_D^- \phi = 1$, then by Eq. (4.2.12) we have $\gamma_D^+ \phi = 1$ and thanks to the fact that K is mass preserving,

$$< \gamma_D^- \phi(r), \gamma_D^- f(r) >_- = < \gamma_D^+ \phi(r), K \gamma_D^- f(r) >_+ \qquad (4.2.26)$$

for any $\gamma_D^- f \epsilon L^{1,-}$, and hence

$$\psi = \gamma_D^- \phi(r) - (PK)^\dagger P \gamma_D^+ \phi(r) = 0. \qquad (4.2.27)$$

Let us denote by λ_D^+ the operator that carries $\gamma_D^- \phi(r)$ into $\gamma_D^+ \phi(r)$ (via $\Lambda\phi = 0$; i.e.,by Eq. (4.2.12), λ_D^+ deposits the value $\gamma_D^- \phi(r)$ taken at a point x of the boundary as a value for $\gamma_D^+ \phi(r)$ on the next intersection with the boundary of the half straight line through x directed and oriented as $-\boldsymbol{\xi}$). Eq. (4.2.27) which holds for $\gamma_D^- \phi = 1$ (and hence $\gamma_D^+ \phi = \lambda_D^+ \gamma_D^- \phi = 1$) then shows that the operator $I - (PK)^\dagger P \lambda_D^+$ does not possess an inverse in $L^{\infty,-}$. Thus Eq. (4.2.24) cannot provide us with a good estimate for the norm of $\gamma_D^- f(r)$ in $L^{1,-}$. Let us then consider for any function ϕ of $L^{\infty,-}$ the decomposition into a constant part

$$P_M \phi = < \phi, M_w^- >_- \; / < 1, M_w^- >_- \qquad (4.2.28)$$

plus the remainder

$$P_O \phi = \phi - P_M \phi. \qquad (4.2.29)$$

All this makes sense, if the boundary has a finite measure. We can now assume that the operator $I - (PK)^\dagger P \lambda_D^+$ has a bounded inverse in the subspace O of the functions having the form $P_O \phi$. Then, by allowing only functions of this kind and taking the supremum with respect to such functions, we obtain the boundedness of the part of $\gamma_D^- f(r)$ which lies in any complete subspace of functions $f \in L^{1,-}$ for which $< P_M \phi, f >_- = 0$. One such subspace is obtained by decomposing any $f \in L^{1,-}$ into $c M_w^- + g$, where c is a factor defined by

$$c = < 1, f >_- \; / < 1, M_w^- >_- \; . \qquad (4.2.30)$$

Then

$$< 1, g >_- = 0. \tag{4.2.31}$$

It is clear that in this way $L^{1,-}$ is decomposed into two subspaces M' and O'; we remark that $< P_M\phi,\, P_{O'}f >_- = 0$, and hence $P_{O'}\gamma_D^- f(r)$ is bounded in $L^{1,-}$.

Thus, although the traces of f may not exist, it makes sense to talk of $P_{O'}\gamma_D^- f(r)$, where $P_{O'}$ is the projector into O'. In order to talk about $\gamma_D^- f(r)$, we must have additional information on f. To this end, it is enough to assume that not only $f \in W^1$, but also $|\boldsymbol{\xi}|^2 f \in L^1$ and $|\boldsymbol{\xi}|^2 \Lambda f \in L^1(D)$. In fact if this holds, then by taking ϕ a function that equals $\mathbf{n}(\mathbf{x})$ on the boundary we obtain through Eq. (4.2.22) (see also Hamdache[29], Lemma 4.3)

$$\|\, |\boldsymbol{\xi}\cdot\mathbf{n}|\gamma_D^- f(r)\, \|_{L^{1,-}} \leq h \,\|\, (1+|\boldsymbol{\xi}|^2) f\, \|_{W^1} \tag{4.2.32}$$

where h is a constant.

One can also prove the following

Theorem 4.2.3. *(See Refs.* 20 *and* 22.*) Let* $f \in W^1, |\boldsymbol{\xi}|^2 f \in L^1, |\boldsymbol{\xi}|^2\Lambda f \in L^1(D)$. *If the boundary condition* (4.1.1) *applies and* $I - (PK)^\dagger P\lambda_D^+$ *has a bounded inverse in the subspace* O *of* $L^{\infty,-}$, *then* $\gamma_D^\mp f \in L^{1,\mp}$.

Theorem 4.2.3 is the result that is needed in order to deal with sufficiently general boundary operators K; Hamdache's[29] results refer, apart from the deterministic conditions of specular and reverse reflection, only to operators with kernels having compact support in $\Re^3 \times \Re^3$ for almost any $\{\mathbf{x}, t\} \in \partial\Omega \times [0, T]$, which excludes practically all the typical cases.

One must, of course, prove that the criterion in Theorem 4.2.3 is actually satisfied by any reasonable boundary condition for sufficiently smooth boundaries. So far an explicit proof has been given[28] for the important case of a boundary diffusing the particles according to a Maxwellian distribution. The proof is based on the fact that, in this case, the inverse operator to be constructed is the identity plus an operator whose range is in the subspace of the functions independent of $\boldsymbol{\xi}$. Then everything is reduced to finding this last part of the operator; this leads to a linear integral equation for a function of $x \in \partial\Omega$. This equation has appeared before in the literature and can be solved in an L^2 framework, by means of Fredholm theorems provided the singularity of the kernel $b(\mathbf{x}, x')$ at $x = x'$ is sufficiently weak. The most general discussion of the abovementioned integral equation is due to Maslova[34], who treated the case in which the boundary is a Lyapunov surface (i.e., essentially, the angle between two neighbouring points x and x' of the surface is less, in absolute value, than $\Lambda|\mathbf{x} - \mathbf{x}'|^\lambda$, with $\Lambda > 0$ and $0 < \lambda \leq 1$ given constants). We can thus prove that Theorem 4.2.3 applies to the case of diffuse reflection on a Lyapunov boundary. For further details we refer to the paper by Cannone and Cercignani[14].

4.3 Properties of the Free-streaming Operator

As in the previous sections, we shall assume that f is assigned at $t = 0$ and satisfies the boundary condition (4.1.1). We first consider the problem

$$(\Lambda + \lambda)f = 0 \qquad \text{in } D \qquad (\lambda \in \Re), \tag{4.3.1}$$

$$\gamma_D^+ f(\mathbf{x}, \boldsymbol{\xi}, t) = K\gamma_D^- f \qquad \text{on } \partial D, \tag{4.3.2}$$

$$f(\mathbf{x}, \boldsymbol{\xi}, 0) = f_0(\mathbf{x}, \boldsymbol{\xi}). \tag{4.3.3}$$

The parameter λ is introduced for the sake of more flexibility when obtaining the estimates; in fact if f solves Eq. (4.3.1–3), then $\hat{f} = e^{\lambda t} f$ satisfies Eqs. (4.3.1–3) with $\lambda = 0$. If the norm of K is (in some space) less than unity, then we can use iteration methods to solve the problem; since, however, we assume that (4.2.3) is true, then the right assumption is $\| K \| = 1$. The boundary will be assumed to be piecewise C^1. We use the notation of Section 2 and set $Y^{p,\pm} = L^p(\Sigma^\pm | \, |\mathbf{n}(\mathbf{x}) \cdot \boldsymbol{\xi}| d\sigma d\boldsymbol{\xi})$. In addition we assume $\| K \| \leq 1$ in $B(Y^{p,-}, Y^{p,+})$ because in this way we can obtain intermediate results, which are useful in the case $\| K \| = 1$. Denote the dual of K by $K^\dagger$. Then for $p \in [1, \infty)$ we have, automatically, $\| K^\dagger \| \leq 1$ in $B(Y^{q,-}, Y^{q,+})$ with $p^{-1} + q^{-1} = 1$. For $p = \infty$ this is an extra assumption (always true in the physically interesting cases). We shall also assume that K does not act on t; hence we may replace $Y^{p,\pm}$ by $L^{p,\pm} = L^p(E^\pm | \, |\mathbf{n}(\mathbf{x}) \cdot \boldsymbol{\xi}| dt d\sigma d\boldsymbol{\xi})$.

The weak solution is defined, as usual, through a sort of Green's formula, which can be established[3] in the same way as (4.2.22):

$$< \gamma_D^- f(r), \gamma_D^- \phi(r) >_- - < \gamma_D^+ f(r), \gamma_D^+ \phi(r) >_+ = (f, (\Lambda - \lambda)\phi) + ((\Lambda + \lambda)f, \phi) \tag{4.3.4}$$

where $< \phi, \psi >_\pm$ are defined as in Eq. (4.2.12). We take as space of test functions

$$W_p^\dagger = \{\phi \in \hat{W}^q | \ \gamma_D^- \phi = K^\dagger \gamma_D^+ \phi, \ \phi(.,T) = 0\} \tag{4.3.5}$$

where $\hat{W}^q$ was defined by Eq. (4.2.18). If f satisfies (4.3.1–3) in a strong sense, then Eq. (4.3.4) gives

$$(f, (\Lambda - \lambda)\phi) = - < f_0, \phi >_{V^+} . \tag{4.3.6}$$

Let us define a weak solution:

Definition 4.3.1. Let $f_0 \in L^p(\Omega \times \Re^3)$. $f \in L^p(D)$ is called a weak solution of (4.3.1–3) if Eq. (4.3.6) holds for any $\phi \in W_p^\dagger$.

Theorem 4.3.1. *If $p \in [1, \infty]$ and $f_0 \in L^p(\Omega \times \Re^3)$, a weak (actually mild) solution $f \in L^p(D)$ exists for $\lambda > 0$ if $\| K \| < 1$. If K carries nonnegative functions into functions of the same kind and f_0 is nonnegative, then f is also nonnegative.*

This theorem can be proved in many ways. Ukai[38] gives a proof that is valid only if $p \in (1, \infty]$. A different strategy is followed in Ref. 22.

One can characterize the weak solutions by the following

Theorem 4.3.2. *(see Refs.* 39 *and* 22*). Any weak solution $f \in L^p(D)$ satisfies:*

(i) $f \in W^p, \qquad (\Lambda + \lambda) f = 0.$

(ii) $f(.,0) = f_0 \in L^p(\Omega \times \Re^3).$

(iii) *If we let $f_\epsilon = \chi_\epsilon f$ (where χ_ϵ is the characteristic function of the set $s(r) \equiv s_+(r) + s_-(r) > \epsilon$), then $\gamma_D^+ f_\epsilon - K\gamma_D^- f_\epsilon \to 0$ ($\epsilon \to \infty$) weakly if $p \in (1,\infty)$ or weak-* if $p = \infty$, in $L^{p,+}$.*

Some estimates for the weak solutions are provided by

Theorem 4.3.3. *When $\| K \| < 1$, the mild solution is unique with the estimates*

$$\lambda p \| f \|^p_{L^p(D)} + (1 - \| K \|^p) \| \gamma^- f \|^p_{L^{p,+}} + \| f(T) \|^p_{L^p(\Omega\times\Re^3)} \leq \| f_0 \|^p_{L^p(\Omega\times\Re^3)} \tag{4.3.7}$$

for $p \in [1,\infty)$ and

$$\| f \|_{L^\infty(D)}, \quad \| \gamma^- f \|_{L^{\infty,+}}, \quad \| f(T) \|_{L^\infty(\Omega\times\Re^3)} \leq \| f_0 \|_{L^\infty(\Omega\times\Re^3)} \tag{4.3.8}$$

for $p = \infty$.

For the proof see Ref. 22.

In the case $\| K \| = 1$ one can prove

Theorem 4.3.4. *When $\| K \| = 1$, if K carries nonnegative functions into functions of the same kind and f_0 is nonnegative, then* (4.3.1–3) *have a mild nonnegative solution $f \in L^p(D)$, with the estimate ($\lambda > 0$):*

$$\| f(.,T) \|_{L^p(\Omega\times\Re^3)} \leq \| f_0 \|_{L^p(\Omega\times\Re^3)} . \tag{4.3.9}$$

Remark. The problem of uniqueness for $\| K \| = 1$ has been solved[5] only with additional conditions on K.

For the proof see Ref. 22.

So far we have assumed $\lambda > 0$. We have already remarked, however, that the constant λ can be removed and thus all the results remain true with some changes in the estimates. In particular one can prove

Corollary 4.3.5. *Theorem* 4.3.4 *is true for $\lambda = 0$ as well.*

Since $f(T) \in L^p(\Omega \times \Re^3)$ by (4.3.9) and since $T > 0$ may be arbitrary, we can introduce the solution operator $U(t)$ ($t \in \Re^+$) which carries $f_0 = f(.,0)$ into $f(.,t)$:

$$U(t) f_0 = f(.,t). \tag{4.3.10}$$

Then it is not hard to prove

Theorem 4.3.6. *If $p \in [1,\infty)$, $U(t)$ is a C_0-semigroup on $L^p(\Omega \times \Re^3)$.*

Remark. The continuity property is lacking for $p = \infty$.

In the sequel we shall need a generalization of these results to the case when the parameter λ in Eq. (4.3.1) is replaced by a nonnegative function $l(t, \mathbf{x}, \boldsymbol{\xi}) \in L^1((0,T) \times \Omega \times \Re^3{}_{\text{loc}})$. Then the above treatment carries through. The main difference arises in the definition of the spaces W^p and $W_p^{\dagger}$ and in the proof of the analogue of Theorem 4.3.1. In fact W^p is now replaced by W_l^p, such that $f \in L^p$ and $(\Lambda + l)f \in L^p$ and $W^{p\dagger}$ is replaced by $W_l^{p\dagger}$, such that $f \in L^p$ and $(\Lambda - l)f \in L^p$. The proof is given in Ref. 22, where one concludes with

Theorem 4.3.7. *When $\| K \| = 1$, if K carries nonnegative functions into functions of the same kind and f_0 is nonnegative, then the problem*

$$(\Lambda + l)f = 0 \qquad \text{in } D \tag{4.3.11}$$

(where $0 \leq l = l(t, \mathbf{x}, \boldsymbol{\xi}) \in L^1((0,T) \times \Omega \times \Re^3_{loc})$) with the boundary and initial conditions (4.3.2–3) has a mild nonnegative solution $f \in L^p(D)$, with the estimate

$$\| f(.,T) \|_{L^p(\Omega \times \Re^3)} \leq \| f_0 \|_{L^p(\Omega \times \Re^3)} \, . \tag{4.3.12}$$

The solution can be written as $U_l(t)f_0$, where, if $p \in [1, \infty)$, $U_l(t)$ is a C_0-semigroup on $L^p(\Omega \times \Re^3)$.

We shall also have to deal with sequences of nonnegative functions $l_k \in L^1((0,T) \times \Omega \times \Re^3_{\text{loc}})$. In this case, if $\{l_k\}$ converges to l in $L^1((0,T) \times \Omega \times \Re^3_{\text{loc}})$, then $\{F_k\}$, where

$$F_k = \int_{-s^-(r)}^{0} l_k(s, \mathbf{x} - \boldsymbol{\xi}(t+s), \boldsymbol{\xi}) ds \tag{4.3.13}$$

is a bounded sequence in $C([0,T], L^1(\Omega \times \Re^3{}_{\text{loc}}))$ and converges for any $t \in R_+$, a.e. in $(\mathbf{x}, \boldsymbol{\xi})$ to

$$F = \int_{-s^-(r)}^{0} l(s, \mathbf{x} - \boldsymbol{\xi}(t+s), \boldsymbol{\xi}) ds. \tag{4.3.14}$$

Associated with the sequence $\{l_k\}$ we have now the sequence of solutions $\{U_{l_k}(t)f_0\}$ (for the sake of simplicity we restrict our attention now to the case $p = 1$), which is pointwise dominated by $U(t)f_0$. Thus $\{U_{l_k}(t)f_0\}$ converges to $U_l(t)f_0$ because of the dominated convergence theorem, and thanks to the fact that all the relations that we need apply (see Ref. 22), we can pass to the limit when we replace l by l_k and let n go to ∞ (in $[0,T]$ for a. e. $(\mathbf{x}, \boldsymbol{\xi})$.

We remark that we can also solve

$$(\Lambda + l)f = g \qquad \text{in } D \qquad (\lambda \in \Re) \tag{4.3.15}$$

with initial and boundary conditions (4.3.2) and (4.3.3), when $g \in L^1((0,T) \times \Omega \times \Re^3_{\text{loc}})$. The solution is

$$f = U_l(t)f_0 + \int_0^t U_l(t-s) g ds. \tag{4.3.16}$$

We also remark that the traces do exist and satisfy Eq. (4.1.1) almost everywhere in $[0,T] \times \partial\Omega \times \Re^3$, because this is true of any function of the form $U_l(\tau)g$, $\tau > 0$.

We finally notice that $\{U_l g^\nu\}$ is an increasing sequence when $\{g^\nu\}$ is such a sequence.

4.4 Existence in a Vessel with an Isothermal Boundary

In order to deal with the existence theorem in a vessel at rest, with constant temperature along the boundary, it is convenient to remark that there is an absolute Maxwellian naturally associated with the problem, i.e., the wall Maxwellian M_w; an exception is offered by specular reflecting boundaries. In the latter case M_w will mean the absolute Maxwellian with zero bulk velocity and total mass and energy equal to the total mass and energy of the gas at time t=0. Eq. (4.1.5) gives

$$\int \boldsymbol{\xi} \cdot \mathbf{n} \gamma_D f \log \gamma_D f d\boldsymbol{\xi} + \beta_w \int \boldsymbol{\xi} \cdot \mathbf{n} |\boldsymbol{\xi}|^2 \gamma_D f d\boldsymbol{\xi} \leq 0 \tag{4.4.1}$$

(a.e. in t and $x \in \partial\Omega$). Then the modified H-functional

$$H = \int f \log f d\boldsymbol{\xi} d\mathbf{x} + \beta_w \int |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi} d\mathbf{x} \tag{4.4.2}$$

will decrease in time, as a consequence of the Boltzmann equation and inequality (4.4.1). Thus H is bounded if bounded initially.

Let us divide the subset of $\Omega \times \Re^3$ where $f < 1$ into two subsets $\Delta^\pm = \{(\mathbf{x}, \boldsymbol{\xi}) : \pm \log f < \mp \beta_w \boldsymbol{\xi}^2/2)\}$. Then (since $-f \log f$ is a growing function in $(0, e^{-1})$ and less than f for $f > e^{-1}$)

$$-\int_{\Delta^+} f \log f d\boldsymbol{\xi} d\mathbf{x} \leq \int f d\boldsymbol{\xi} d\mathbf{x} + \beta_w \int \boldsymbol{\xi}^2 \exp[-\beta_w \boldsymbol{\xi}^2/2] d\boldsymbol{\xi} d\mathbf{x} \leq C \tag{4.4.3}$$

and in Δ^-,

$$-\int_{\Delta^-} f \log f d\boldsymbol{\xi} d\mathbf{x} \leq [\beta_w/2] \int \boldsymbol{\xi}^2 f d\boldsymbol{\xi} d\mathbf{x} \tag{4.4.4}$$

Then Eq. (4.4.2) implies that both $\int f |\log f| d\boldsymbol{\xi} d\mathbf{x}$ and $\int |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi} d\mathbf{x}$ are separately bounded in terms of the initial data. It is then easy to prove that the mass and entropy relations take on the following form:

$$\int f(\cdot, t) d\boldsymbol{\xi} d\mathbf{x} = \int f(., 0) d\boldsymbol{\xi} d\mathbf{x}, \tag{4.4.5}$$

$$\begin{aligned} &\int f \log f(., t) d\boldsymbol{\xi} d\mathbf{x} + \beta_w \int |\boldsymbol{\xi}|^2 f(., t) d\boldsymbol{\xi} d\mathbf{x} + \int_0^t \int e(f)(\cdot, s) d\boldsymbol{\xi} d\mathbf{x} ds \\ &\leq \int f \log f(\cdot, 0) d\boldsymbol{\xi} d\mathbf{x} + \beta_w \int |\boldsymbol{\xi}|^2 f(., 0) d\boldsymbol{\xi} d\mathbf{x} \end{aligned} \tag{4.4.6}$$

where

$$e(f)(\mathbf{x},\boldsymbol{\xi},t) = \frac{1}{4}\int_{\Re^3}\int_{S^+}(f'f'_* - ff_*)\log(f'f'_*/ff_*)B(|\mathbf{V}|,\mathbf{V}\cdot\mathbf{n})d\boldsymbol{\xi}_* d\mathbf{n}. \quad (4.4.7)$$

The theorem that we shall state now was first discussed by Hamdache[29], but here we shall rather refer to the previously quoted paper by Arkeryd and Cercignani[3], which, although devoted to the case of non-isothermal boundaries, contains a slightly different proof of Hamdache's theorem, with an extension to more general boundary conditions, to a more detailed study of the boundary behavior, and for the full class of collision operators of the Di Perna and Lions[26] existence context. As hinted at in Section 2, the proof uses the equivalent concepts of exponential, mild, and renormalized solutions as defined by DiPerna and Lions[26] and such solutions will be found as limits of functions solving truncated equations. This existence theorem reads as follows.

Theorem 4.4.1. *Let $f^0 \in L^1(\Omega \times \Re^3)$ be such that*

$$\int f^0(1+|\boldsymbol{\xi}|^2)d\boldsymbol{\xi}d\mathbf{x} < \infty, \qquad \int f^0|\log f^0|d\boldsymbol{\xi}d\mathbf{x} < \infty. \quad (4.4.8)$$

Then there is a mild solution $f \in C(\Re_+, L^1(\Omega \times \Re^3))$ of the Boltzmann equation such that $f(.,0) = f^0$, which also satisfies relations (4.4.5) *and* (4.4.6).

For a sketch of the proof see Ref. 22.

We are now in a position to discuss the boundary conditions satisfied by the solutions. These boundary conditions have been left unspecified so far. In fact, the previous theorem only says that f is a mild solution (and hence a renormalized solution) of the Boltzmann equation but gives no indication whether this solution satisfies the boundary conditions. This would be automatic if f were an ordinary weak solution. The only result proved, by Hamdache[29] and, in a more explicit way, by Arkeryd and Cercignani[3], is that Eq. (4.1.1) is replaced by an inequality. Following these papers one can prove

Theorem 4.4.2. *There is a solution as in Theorem* 4.4.1*, which satisfies*

$$\gamma_D^+(f) \geq K(\gamma_D^- f) \quad \text{a. e. on } E^+ \quad . \quad (4.4.9)$$

Remark. If the traces of the solutions are in $L^{1\pm}$ (as in the case of Maxwellian diffusion at the boundary), and if $Q(f,f)$ belongs to $L^1(D)$, then there is equality in (4.4.9).

4.5 The Results of Arkeryd and Maslova

In this section we study the results presented by Arkeryd and Maslova[20]. They introduce a class of boundary operators for which (4.3.2), (4.2.1–3) hold, by restricting the adjoint operator K^*, but are able to avoid the cutoff for large velocities.

A better control of mass, energy and entropy for the distributions emerging from the wall are provided by the following conditions:

$$\text{There exists } K_2 > 0 \text{ such that } K^*|\boldsymbol{\xi}\cdot n(x)| \geq K_2 \quad \text{(spreading condition).} \tag{4.5.1}$$

$$\text{There exists } K_3 \leq \infty \text{ such that } K^*|\boldsymbol{\xi}|^2 \leq K_3 \quad \text{(energy condition).} \tag{4.5.2}$$

$$\begin{gathered}\text{There exists } K_4 < \infty \text{ and } \alpha \in [0,1) \text{ such that, for every } f \in L^1(\Gamma^-) \text{ with } f \geq 0,\\ \text{it holds } < Kf, \log(Kf/(f,1)_-) >_+ - \alpha\hat{H}^- \leq K_4(q_2^- + q) \quad \text{(entropy condition).}\end{gathered} \tag{4.5.3}$$

Here

$$\begin{gathered}\hat{H}^- =< f, \log(f/(f,1)_-) >_- \qquad q_j^\pm =< f, |\boldsymbol{\xi}|^j >_\pm,\\ q =< f, |\boldsymbol{\xi}\cdot\mathbf{n}| >_+ + < f, |\boldsymbol{\xi}\cdot\mathbf{n}| >_- .\end{gathered} \tag{4.5.4}$$

These conditions are reasonable for a linear operator, except for (4.5.3), which appears a bit unusual, since it is nonlinear, albeit homogeneous of first degree in f. Later in this section we shall discuss how to dispense with that condition by using Lemma 4.2.1 in a suitable way.

The other conditions have the following role (Lemma 4.1 of Arkeryd and Maslova[20]):

1. Eq. (4.5.1) (together with a proper use of momentum balance) gives a control on the mass flow hitting the boundary.
2. Eq. (4.5.2) (together with 1)) gives a control on q_2^+.
3. Using 1) and 2) together with energy balance one obtains an a priori bound upon the energy without using the entropy estimates.

At this point Arkeryd and Maslova[20] use Eq. (4.5.3) to bound the entropy and the entropy source. They also obtain bounds on $< f, |\log(f/(f,1)_-)| >_\pm$ which are related to entropy flows. To bound the latter, however, one should remove the denominator $(f,1)_-$, which does not appear to be an easy matter.

The following lemma holds[20].

Lemma 4.5.1. *Assume Eqs.* (4.2.2–3) *and* (4.5.1–3), *together with*

$$(f_0, \log f_0) \in L^1(\Omega), \tag{4.5.5}$$

$$(Q, \log f) \leq 0, \quad (Q, \psi) = 0 \quad \textit{for } \psi = 1, \boldsymbol{\xi}, |\boldsymbol{\xi}|^2. \tag{4.5.6}$$

Then f satisfies the inequality

$$- < Q, \log f > + H(T) + < f, |\log(f/(f,1)_-)| >_\pm \leq C(T), \tag{4.5.7}$$

with $C(T) > 0$ depending only on f_0 and on K_2, K_3, K_4.

Having these a priori bounds they proceed more or less as in the paper by Arkeryd and Cercignani[15], the main change being that they prefer to avoid the semigroups that were used there, and finally arrive at

Theorem 4.5.2. *Assume that*

$$(1+|\boldsymbol{\xi}|^2)f_0, \quad f_0 \log f_0 \in L^1(\Omega \times R^3), \qquad f_0 \geq 0,$$

and Eqs. (4.5.1–3)*. Then there exists an exponential solution of* (4.1.1–3) *satisfying*

$$f \in C([0,T], L^1(\Omega \times R^3)_{)}, \quad f \geq 0, \quad < f, 1 >_t = < f_0, 1 >_0;$$

$$(1+|\boldsymbol{\xi}|^2)\gamma^{\pm} f \in L^{1\pm} \ ; \tag{4.5.8}$$

$$\sup_{t \leq T}[< f, \ln f >_t + < f, |\boldsymbol{\xi}|^2 >_t] + < e(f), 1 > \leq C(T). \tag{4.5.9}$$

Here

$$e(f) = \frac{1}{4}\int_{R^3}\int_{B+}(f'f'_* - ff_*)\log\frac{f'f'_*}{ff_*}B(\boldsymbol{\xi} - \boldsymbol{\xi}_*, \mathbf{n})d\boldsymbol{\xi}_* d\mathbf{n}.$$

It is also possible to prove a result which relaxes one of the assumptions of Arkeryd and Maslova[20] and a generalization to the case of moving boundaries. In fact, Lemma 4.5.1 and (as a consequence) Theorem 4.5.2 hold without assuming (4.5.3), but only the compatibility with a Maxwellian, Eq. (4.2.4). The inequality of Darrozès and Guiraud[16] then holds. One can prove

Lemma 4.5.3. *Assume Eqs.* (4.2.2–4) *and* (4.5.1–2) *, together with* $\beta_w \leq C_o(T)$ *and*

$$(f_0, \log f_0) \in L^1(\Omega), \tag{4.5.10}$$

$$(Q, \log f) \leq 0, \quad (Q, \psi) = 0 \quad \textit{for } \psi = 1, \boldsymbol{\xi}, |\boldsymbol{\xi}|^2. \tag{4.5.11}$$

Then f *satisfies the inequality*

$$- < Q, \log f > + H(T) \leq C(T), \tag{4.5.12}$$

with $C(T) > 0$ *depending only on* f_0 *and on* K_2, K_3.

Proof. Using Green's formula[13,29,20] and approximation,

$$- < Q, \log f > + H(T) + < f, \log f >_- \leq H(0) + < f, \log f >_+ . \tag{4.5.13}$$

Because of Lemma 4.5.1 this becomes

$$- < Q, \log f > + H(T) + < \beta_w f, |\boldsymbol{\xi}|^2 >_+ \leq H(0) + < \beta_w f, |\boldsymbol{\xi}|^2 >. \tag{4.5.14}$$

Thanks to the fact that β_w is bounded, energy balance now gives (Lemma 4.1 of Arkeryd and Maslova[20]) that the last term is bounded by some $C(T)$. Hence

$$- < Q, \log f > + H(T) + < \beta_w f, |\boldsymbol{\xi}|^2 >_+ \leq C(T)$$

which implies that the three quantities on the left-hand side are separately bounded. In particular, Eq. (4.5.12) follows. □

The only part of the thesis of Lemma 4.5.1 that does not follow from the new assumptions is the boundedness of the entropy flows $< f, |\log(f/(f,1)_-)| >_\pm$. This part of the lemma is never used in the proof of Theorem 4.5.2 and thus we can prove

Theorem 4.5.4. *Assume that*

$$(1+|\boldsymbol{\xi}|^2)f_0, \quad f_0 \log f_0 \in L^1(\Omega \times R^3), \qquad f_0 \geq 0,$$

and Eqs. (4.2.2–4) *and* (4.5.1–2). *Then there exists an exponential solution of* (4.1.1–3) *satisfying*

$$f \in C([0,T], L^1(\Omega \times R^3)), \quad f \geq 0, \quad < f, 1 >_t = < f_0, 1 >_0;$$

$$(1+|\boldsymbol{\xi}|^2)\gamma^\pm f \in L^{1\pm} \; ; \tag{4.5.15}$$

$$\sup_{t \leq T}[< f, \ln f >_t + < f, |\boldsymbol{\xi}|^2 >_t] + < e(f), 1 > \leq C(T), \tag{4.5.16}$$

where $e(f)$ *is given by Eq.* (4.5.10).

Remark. The above result applies also to the inhomogeneous boundary condition

$$\gamma^+ f(x, \boldsymbol{\xi}, t) = \alpha f_+ + (1-\alpha)K\gamma^- f \quad (0 \leq \alpha \leq 1) \tag{4.5.17}$$

where $f_+ \geq 0$ is assigned.

We pass now to problems with moving boundaries. The main difference is that in Eq. (4.1.2) E^+ varies with time, because $\partial\Omega$ does. As remarked in Section 2, all the relations concerning the kernel K hold in the reference frame of the wall. Then, when the Maxwellian M_w has a drift velocity $\mathbf{u}_w$, if we want to adopt a reference frame, with respect to which the wall moves, then $\boldsymbol{\xi}$ must be replaced by $\boldsymbol{\xi} - \mathbf{u}_w$. In particular, the indices + and − refer now to $(\boldsymbol{\xi} - \mathbf{u}_w) \cdot \mathbf{n} > 0$ and $(\boldsymbol{\xi} - \mathbf{u}_w) \cdot \mathbf{n} < 0$, respectively.

When we integrate the Boltzmann equation to obtain a priori inequalities, we obtain a factor $(\boldsymbol{\xi} - \mathbf{u}_w) \cdot \mathbf{n}$ in place of $\boldsymbol{\xi} \cdot \mathbf{n}$, so that most of the changes compensate. The main difference arises in the entropy inequality, where a factor $|\boldsymbol{\xi} - \mathbf{u}_w|^2$ appears in place of simply $\boldsymbol{\xi}^2$. the extra terms can be easily controlled, however, by means of the momentum balance equation (after scalar multiplication by a smooth vector-valued function $\mathbf{u}(x,t)$, which reduces to $\mathbf{u}_w$ on the wall).

Then we have the following

Corollary 4.5.5. *Theorem* 4.5.4 *holds in the presence of moving walls as well.*

4.6 Rigorous Proof of the Approach to Equilibrium

Discussions of equilibrium states in kinetic theory are as old as the theory itself; actually these states were discussed even before the basic evolution equation of the theory, i.e., the Boltzmann equation, was formulated. The recent work on the mathematical aspects of kinetic theory has led to new results on this problem as well.

The aim of this section is to discuss the trend to equilibrium, following the approach of Desvillettes[25] and Cercignani[19], which is based on a remark by DiPerna and Lions[27]. The main result is the following:

Theorem 4.6.1. *Let $f(\mathbf{x}, \boldsymbol{\xi}, t)$ be the solution of the Boltzmann equation, with initial data $f_0(\mathbf{x}, \boldsymbol{\xi})$ such that*

$$f_0 \geq 0; \qquad \int_\Omega \int_{\Re^3} f_0(\mathbf{x}, \boldsymbol{\xi})(1 + |\boldsymbol{\xi}|^2 + |\log f_0(\mathbf{x}, \boldsymbol{\xi})|) d\mathbf{x} d\boldsymbol{\xi} < +\infty. \tag{4.6.1}$$

Let f also satisfy the boundary condition (4.1.1)*,where the kernel is such that Eqs.* (4.1.2–4) *hold (M_w being a constant and uniform Maxwellian). Then, for every sequence t_n going to infinity, there exist a subsequence t_{n_k} and a local Maxwellian $M(\mathbf{x}, \boldsymbol{\xi}, t)$ such that $f_{n_k}(\mathbf{x}, \boldsymbol{\xi}, t) = f(\mathbf{x}, \boldsymbol{\xi}, t_{n_k} + t)$ converges weakly in $L^1(\Omega \times \Re^3 \times [0, T])$ to $M(\mathbf{x}, \boldsymbol{\xi}, t)$ for any $T > 0$. Moreover M satisfies the free transport equation*

$$\frac{\partial M}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial M}{\partial x} = 0 \tag{4.6.2}$$

and the boundary condition (4.1.1)*.*

For the proof see Refs. 25, 19 and 22.

Theorem 4.6.1 tells us that the solutions of the Boltzmann equation with the boundary conditions (4.1.1) behave (in the case of a boundary at constant temperature) as Maxwellians satisfying the free transport equation, Eq. (4.6.2). These Maxwellians have been well known since Boltzmann[13] and were already discussed in Chapter 1. They have the following form:

$$M = \exp[a_0 + b_0 \cdot \boldsymbol{\xi} + c_0|\boldsymbol{\xi}|^2 + d_0|\mathbf{x} - \boldsymbol{\xi}t|^2 + e_0 \cdot (\mathbf{x} - \boldsymbol{\xi}t) + f_0 \cdot (\mathbf{x} \wedge \boldsymbol{\xi})] \tag{4.6.12}$$

where $a_0, c_0, d_0 \in \Re$ and $b_0, e_0, f_0 \in \Re^3$ are constants. Now if we impose the condition that $M(\mathbf{x}, ., t)$ is an L^1 function for any $t \geq 0$, we see that c_0 must be negative and d_0 nonpositive. We exclude now from our considerations the cases in which the kernel K is a delta function; in fact, the only significant situations in which a Dirac delta occurs are exceptional and can easily be treated in detail as shown by Desvillettes[25]. In the other cases, there is only one Maxwellian which is compatible with the boundary conditions, i.e., a Maxwellian with no drift and constant temperature; this immediately implies that b_0, d_0, e_0, f_0 are zero. Hence M is a uniform Maxwellian, which coincides with M_w. Thus we have the following result, embodying the results of Desvillettes[25] and Cercignani[19]:

Theorem 4.6.2. *The Maxwellian M in Theorem* 4.6.1 *is uniform, with the exception of specularly reflecting boundaries having rotational symmetry about an axis ℓ. In the latter case the Maxwellian M might describe a solid body rotation of the gas about ℓ.*

L. Arkeryd[1] has proved that f actually tends to a Maxwellian in a strong sense for a periodic box, but his argument, based on nonstandard analysis, works in other cases as well. Subsequently P.-L. Lions[33] obtained the same result without resorting to nonstandard analysis.

4.7 Perturbations of Equilibria

Let us consider again the initial-boundary value problem for the Boltzmann equation

$$\Lambda f = Q(f, f) \qquad \text{in } D, \tag{4.7.1}$$

$$\gamma_D^+ f(\mathbf{x}, \boldsymbol{\xi}, t) = K\gamma_D^- f \qquad \text{on } \partial D^+, \tag{4.7.2}$$

$$f(\mathbf{x}, \boldsymbol{\xi}, 0) = f_0(\mathbf{x}, \boldsymbol{\xi}). \tag{4.7.3}$$

Let $U(t)$ be as in (4.6.15) ($\lambda = 0$). Then the initial-boundary value problem reduces to solving the integral equation

$$f(t) = U(t)f_0 + \int_0^t U(t-s)Q(f(s), f(s))ds. \tag{4.7.4}$$

It is easy to prove local existence of this equation in several spaces, typically:

$$X_{\alpha,\beta} = \{f|\ (1 + |\boldsymbol{\xi}|^2)^{\alpha/2} \exp(-\beta|\boldsymbol{\xi}|^2) f \in L^\infty(\Omega \times \Re^3)\} \tag{4.7.5}$$

with norm

$$\| f \|_{\alpha,\beta} = \| (1 + |\boldsymbol{\xi}|^2)^{\alpha/2} \exp(-\beta|\boldsymbol{\xi}|^2) f \|_{L^\infty(\Omega\times\Re^3)} . \tag{4.7.6}$$

A case in which one can say a lot more about the solutions of initial-boundary value problems is the case when the data are compatible with a solution close to a uniform Maxwellian distribution M. Then techniques akin to those of Chapter 3 can be used. To this end, let us introduce the perturbation h such that

$$f = M + M^{1/2} h \tag{4.7.7}$$

and first assume that M coincides with the wall Maxwellian, so that Eq. (4.1.4) is satisfied by M. Eqs. (4.7.1–3) can then be rewritten in the following way:

$$\Lambda f = Lh + \Gamma(h, h) \qquad \text{in } D, \tag{4.7.8}$$

$$\gamma_D^+ h(\mathbf{x}, \boldsymbol{\xi}, t) = \hat{K}\gamma_D^- h \qquad \text{on } \partial D, \tag{4.7.9}$$

$$h(\mathbf{x}, \boldsymbol{\xi}, 0) = h_0(\mathbf{x}, \boldsymbol{\xi}) \tag{4.7.10}$$

where L and Γ are the same as in Chapter 3 (see Eqs. (3.1.4) and (3.1.5)), while

$$\hat{K} = M^{-1/2} K M^{1/2} \tag{4.7.11}$$

Now the global solution can be found by the same technique used in Chapter 3, provided the linearized operator

$$B = -\boldsymbol{\xi} \cdot \partial/\partial \mathbf{x} + L \tag{4.7.12}$$

with the boundary conditions (4.7.9) generates a semigroup $T(t)$ with a nice decay.

In the previous chapter, we have met two different types of decay of the semigroup $T(t)$. One of them occurs in the pure initial value problem in $\Re^3$ and the other in the same problem for T^3. We may expect that these two types of result also apply in the presence of boundary conditions: the first of them with a decay like $t^{-\alpha}(\alpha > 0)$ should apply to unbounded domains, while the second, with an exponential decay, should apply to bounded domains.

There are several papers dealing with the proofs of the behaviors conjectured above. The case of a bounded domain has been considered by Guiraud[28] in the case of diffuse reflection and by Shizuta and Asano[37] in the case of specular reflection, both assuming that Ω is convex. The case of unbounded domains exterior to a bounded convex obstacle was treated by several Japanese authors[38,40]. Here it will be dealt with in Section 8 after having studied the corresponding steady flow problem .

4.8 A Steady Flow Problem

We shall now deal with the steady flow of a gas past an obstacle $\mathcal{O}$ whose exterior will be denoted by Ω. At space infinity the distribution function will be a drifting Maxwellian $M_{\mathbf{v}}$. Then the distribution function f satisfies

$$\boldsymbol{\xi} \cdot \partial f/\partial \mathbf{x} = Q(f, f) \qquad \text{in } V, \tag{4.8.1}$$

$$\gamma_D^+ f(\mathbf{x}, \boldsymbol{\xi}) = K \gamma_D^- f \qquad \text{on } \partial V, \tag{4.8.2}$$

$$f(\mathbf{x}, \boldsymbol{\xi}) \to M_{\mathbf{v}}(\boldsymbol{\xi}) = \rho(2\pi/\beta)^{-3/2} \exp(-\beta|\boldsymbol{\xi} - \mathbf{v}|^2) \qquad (|\mathbf{x}| \to \infty). \tag{4.8.3}$$

We remark that $M_{\mathbf{v}}$ ($\mathbf{v} \neq 0$) is not, in general, a solution of (4.8.1–3), because it violates the boundary condition (4.8.2). Since, however, it is a solution of the problem when $\mathbf{v} = 0$, we can expect the solution to be close to $M_{\mathbf{v}}$ when $\mathbf{v}$ is small.

This conjecture has been exploited and proved in a paper by Ukai and Asano[41], to which we shall refer in the sequel.

Since, in analogy with what is discussed in Chapter 3 for the pure initial value problem, the basic technique is to show that the solution is a small perturbation of $M_{\mathbf{v}}$, we let

$$f = M_{\mathbf{v}} + M_w^{1/2} h \tag{4.8.4}$$

where M_w is the wall Maxwellian. We also assume that the temperatures β and β_w of $M_{\mathbf{v}}$ and M_w are close in the sense that $|\beta - \beta_w| \leq \eta|\mathbf{v}|$ with some $\eta \geq 0$.

In terms of h, Eqs. (4.8.1–3) read as follows:

$$\boldsymbol{\xi} \cdot \partial h/\partial \mathbf{x} = L_{\mathbf{v}} h + \Gamma(h,h) \qquad \text{in } V, \tag{4.8.5}$$

$$\gamma_D^+ h(\mathbf{x},\boldsymbol{\xi}) = \hat{K}\gamma_D^- h + s_{\mathbf{v}} \qquad \text{on } \partial V, \tag{4.8.6}$$

$$h(\mathbf{x},\boldsymbol{\xi}) \to 0 \qquad (|\mathbf{x}| \to \infty) \tag{4.8.7}$$

where

$$L_{\mathbf{v}} h = 2M_w^{-1/2} Q(M_{\mathbf{v}}, M^{1/2} h) \tag{4.8.8}$$

and Γ and $\hat{K}$ are as before, while

$$s_{\mathbf{v}} = M_w^{-1/2}(K\gamma_D^- M_{\mathbf{v}} - \gamma_D^+ M). \tag{4.8.9}$$

We remark that $L_{\mathbf{v}}$ is not self-adjoint in $L^2(\Re^3_{\boldsymbol{\xi}})$ when $\mathbf{v} \neq 0$.

Let $B_{\mathbf{v}}$ be the linearized Boltzmann operator

$$B_{\mathbf{v}} = -\boldsymbol{\xi} \cdot \partial/\partial \mathbf{x} + L_{\mathbf{v}} \qquad \text{in } V \tag{4.8.10}$$

with the boundary conditions (4.8.7) and

$$\gamma_D^+ h(\mathbf{x},\boldsymbol{\xi}) = \hat{K}\gamma_D^- h \qquad \text{on } \partial V \tag{4.8.11}$$

and assume that it has an inverse $B_{\mathbf{v}}^{-1}$. Then Eqs. (4.8.5–7) are equivalent to

$$h + B_{\mathbf{v}}^{-1}\Gamma(h,h) = \phi_{\mathbf{v}} \tag{4.8.12}$$

where $\phi_{\mathbf{v}}$ is a solution of the linear steady flow problem

$$\boldsymbol{\xi} \cdot \partial \phi/\partial \mathbf{x} = L_{\mathbf{v}} \phi \qquad \text{in } V, \tag{4.8.13}$$

$$\gamma_D^+ \phi(\mathbf{x},\boldsymbol{\xi}) = \hat{K}\gamma_D^- \phi + s_{\mathbf{v}} \qquad \text{on } \partial V, \tag{4.8.14}$$

$$\phi(\mathbf{x},\boldsymbol{\xi}) \to 0 \qquad (|\mathbf{x}| \to \infty). \tag{4.8.15}$$

Once $B_{\mathbf{v}}^{-1}$ and $\phi_{\mathbf{v}}$ have been shown to exist, we can solve Eq. (4.8.12) by the implicit function theorem (see below). A delicate problem is posed by the existence of $B_{\mathbf{v}}^{-1}$. As we shall see, $0 \in \sigma(B_{\mathbf{v}})$ and thus $B_{\mathbf{v}}^{-1}$ does not exist in $L^2(V)$. By means of the so-called "principle of limiting absorption", familiar in scattering theory, it is possible, however, to find $B_{\mathbf{v}}^{-1}$ (in another function space) as a limit of $(B_{\mathbf{v}} - \lambda I)^{-1}$ as $\lambda \to 0$.

To illustrate the method, let us first consider $B_{\mathbf{v}}$ 3 in the special case $\Omega = \Re^3$. Then, as in Chapter , it is enough to study the Fourier-transformed operator $B_{\mathbf{v}}(\mathbf{k}) = -i\mathbf{k} \cdot \boldsymbol{\xi} + L_{\mathbf{v}}$. $L_{\mathbf{v}}$ has the same properties as L ($= L_{\mathbf{v}}$ for $v = 0$) except self-adjointness. In particular,

$$L_{\mathbf{v}} = -\nu_{\mathbf{v}}(\boldsymbol{\xi}) + K_{\mathbf{v}} \tag{4.8.16}$$

where $\nu_{\mathbf{v}} = \nu(\boldsymbol{\xi}-\mathbf{v})$ and $K_{\mathbf{v}}$ is an integral operator to which Theorem 3.2.4 applies, continuously in $\mathbf{v}$. Let L^2, L_r^∞ be defined in Section 3.2 and $k_0, \sigma_0, \mu_j(\kappa), S_1[\kappa]$ as in Theorem 3.3.6, and set

$$\Sigma(a,\sigma) = \{\lambda : \mathrm{Re}(\lambda) \geq -\sigma; -\mathrm{Re}(\lambda) \leq a|\mathrm{Im}(\lambda)|^2\}. \tag{4.8.17}$$

It is then possible to prove the following

Theorem 4.8.1. *Define $B_{\mathbf{v}}$ in $L^2(\Re^3_{\mathbf{x}} \times \Re^3_{\boldsymbol{\xi}})$ with the maximal domain. Then, for any $v_0 \geq 0$, there is an $a_0 > 0$ such that for all $\mathbf{v} \in S_1[v_0]$, the following holds:*

$$\rho(B_{\mathbf{v}}) \supset \Sigma(a_0,\sigma_0)\backslash\{0\}, \qquad 0 \in \sigma(B_{\mathbf{v}}), \tag{4.8.18}$$

$$(\lambda I - B_{\mathbf{v}})^{-1} = \sum_{j=0}^{5} U_j(\lambda,\mathbf{v}), \tag{4.8.19}$$

for all $\lambda \in \Sigma(a_0,\sigma_0)\backslash\{0\}$, where for $0 \leq j \leq n+1$,

$$U_j(\lambda,\mathbf{v}) = \mathcal{F}_x^{-1}\chi(k)(\lambda - \lambda_j(\mathbf{k},\mathbf{v}))^{-1}P_j(\mathbf{k},\mathbf{v})\mathcal{F}_x,$$

$$\chi(\mathbf{k}) = 1 \quad (\mathbf{k} \in S_1[\kappa_0]), \qquad \chi(\mathbf{k}) = 0 \quad (\mathbf{k} \notin S_1[\kappa_0]),$$

$$\lambda_j(\mathbf{k},\mathbf{v}) = \mu_j(|\kappa|) + i\mathbf{k}\cdot\mathbf{v},$$

$$P_j(\mathbf{k},\mathbf{v}) \in B^0(S_1[\kappa_0] \times S_1[v_0]; \mathbf{B}(L^2, L_r^\infty)), \qquad r \geq 0 \tag{4.8.20}$$

while for $j = 5$,

$$U_5(\lambda,\mathbf{v}) \in B^0(\Sigma(a_0,\sigma_0) \times S_1[v_0]; \mathbf{B}(L^2(\Re^3_x \times \Re^3_{\boldsymbol{\xi}})). \tag{4.8.21}$$

Further, the operators U_j are mutually orthogonal and the $P_j's$ are mutually orthogonal projectors of L^2 with $P_j(\mathbf{k},0) = P_j(\mathbf{k}), \sum_j P_j(0,\mathbf{v}) = P_{\mathbf{v}} = P_0$. Here $U \in B^0(P;V)$ means that U varies in V and is uniformly bounded with respect to parameters varying in set P.

For the proof we refer to the original paper by Ukai and Asano[41].

According to Eq. (4.8.21), $U_5(0,\mathbf{v})$ is a bounded operator, whereas, since $[\lambda_j(\mathbf{k},\mathbf{v})]^{-1}$ has a singularity at $k = 0$ as seen from the asymptotic expansion of $\mu_j(\kappa)$ given in Theorem 3.3.6, $U_j(0,\mathbf{v}), 0 \leq j \leq 4$, are unbounded in $L^2(\Re^3_x \times \Re^3_{\boldsymbol{\xi}})$. However, since this singularity is integrable, $U_j(\lambda,\mathbf{v})$ can be made continuous at $\lambda = 0$ (and, hence, $U_j(0,\mathbf{v})$ is bounded), if the domain and range spaces are chosen appropriately. This is the principle of limiting absorption. In order to arrive at a more precise statement, we set

$$L_r^{p,s} = L_r^{p,s}(\Re^3_{\mathbf{x}} \times \Re^3_{\boldsymbol{\xi}}) = \{h = h(\mathbf{x},\boldsymbol{\xi}) : (1+|\boldsymbol{\xi}|^2)^{r/2}h \in L^s(\Re^3_{\boldsymbol{\xi}}; L^p(\Re^3_{\mathbf{x}}))\}. \tag{4.8.22}$$

Then one can prove the following.

Theorem 4.8.2. *Let* $1 \le q \le 2 \le p \le \infty$, $\theta \in [0,1)$, $m = 0,1$ *with*

$$q^{-1} - p^{-1} > (2-m)/(3+\theta). \tag{4.8.23}$$

Then for $0 \le j \le n+1$,

$$|\mathbf{v}|^\theta U_j(\lambda, \mathbf{v})(I - P_j(0,\mathbf{v}))^m \in B^0(\Sigma(a_0,\sigma_0) \times S_1[v_0]; \mathbf{B}(L_0^{q,2}, L_r^{p,\infty})). \tag{4.8.24}$$

For the proof see Ref. 22.

In order to pass from the case of $\Re^3_{\mathbf{x}}$ to the complement Ω of an obstacle $\mathcal{O}$ in $\Re^3_{\mathbf{x}}$, it is required to solve

$$\lambda h + \boldsymbol{\xi} \cdot \partial h/\partial \mathbf{x} + \nu_{\mathbf{v}} h = 0 \qquad \text{in } V, \tag{4.8.25}$$

$$\gamma_D^+ h(\mathbf{x}, \boldsymbol{\xi}) = s \qquad \text{on } \partial V, \tag{4.8.26}$$

$$h(\mathbf{x}, \boldsymbol{\xi}) \to 0 \qquad (|x| \to \infty), \tag{4.8.27}$$

for a given $s \in Y^{p,+} = L^p(\Sigma^+ |\ |\mathbf{n}(\mathbf{x}) \cdot \boldsymbol{\xi}| d\sigma d\boldsymbol{\xi})$. Assume

$$\mathcal{O} \text{ is a bounded convex domain and } \partial\mathcal{O} = \partial\Omega \text{ is piecewise } C^2. \tag{4.8.28}$$

Then (4.8.25–28) can be easily (and explicitly) solved; denote the solution by $h = R_{\mathbf{v}}(\lambda)s$, where $R_{\mathbf{v}}(\lambda)$ is the solution operator. Let $\mathcal{E}$ be the operator extending an operator A from V to $\Re^3_{\mathbf{x}} \times \Re^3_{\boldsymbol{\xi}}$ by letting $\mathcal{E}A$ be zero in V^c and $\mathcal{R}$ the restriction operator from $\Re^3_{\mathbf{x}} \times \Re^3_{\boldsymbol{\xi}}$ to V. Let also henceforth $B^\infty_{\mathbf{v}}$ denote the Boltzmann operator in $\Re^3_x \times \Re^3_{\boldsymbol{\xi}}$, in order to distinguish it from the Boltzmann operator $B_{\mathbf{v}}$ in V. Further, set

$$\overline{K} = \gamma_D^+ - \hat{K}\gamma_D^- \tag{4.8.29}$$

and

$$T_{\mathbf{v}}(\lambda) = \overline{K}\mathcal{R}(\lambda I - B^\infty_{\mathbf{v}})^{-1}\mathcal{E}K_{\mathbf{v}}R_{\mathbf{v}}(\lambda). \tag{4.8.30}$$

After some manipulations we can write the resolvent $(\lambda I - B_{\mathbf{v}})^{-1}$ in an explicit fashion[41]:

$$\begin{aligned}(\lambda I - B_{\mathbf{v}})^{-1} &= \mathcal{R}(\lambda I - B^\infty_{\mathbf{v}})^{-1}\mathcal{E} + S_{\mathbf{v}}(\lambda)(I - T_{\mathbf{v}}(\lambda))^{-1}\overline{K}(\lambda I - B^\infty_{\mathbf{v}})^{-1}\mathcal{E}S_{\mathbf{v}}(\lambda)\\ &= R_{\mathbf{v}}(\lambda) + \mathcal{R}(\lambda I - B^\infty_{\mathbf{v}})^{-1}\mathcal{E}K_{\mathbf{v}}R_{\mathbf{v}}(\lambda)\\ &= (\gamma_D^+\mathcal{R}(\lambda I - B^{\infty\dagger}_{\mathbf{v}})^{-1}\mathcal{E})^\dagger.\end{aligned} \tag{4.8.31}$$

Originally, this representation formula is obtained in $L^2(V)$ for $\lambda \in \rho(B^\infty_{\mathbf{v}}) \cap \rho(B_{\mathbf{v}})$ and $1 \in \rho(T_{\mathbf{v}}(\lambda))$, but can be used to define $(\lambda I - B_{\mathbf{v}})^{-1}$ in other spaces as far as the right-hand side makes sense. A crucial point is the existence of $(I - T_{\mathbf{v}}(\lambda))^{-1}$, which is guaranteed by the following

Lemma 4.8.3. *Let* $p \in [2,\infty], r > 3(p-2)/(2p)$. *Then, there are positive constants* a_1, v_1, σ_1 *such that*

$$(I - T_{\mathbf{v}}(\lambda))^{-1} \in B^0(\Sigma(a_1,\sigma_1) \times S_1[v_1]; \mathbf{B}(Y_r^{p,+})), \tag{4.8.32}$$

where $Y_r^{p,+} = \{h : (1 + |\boldsymbol{\xi}|^2)^{r/2} u \in Y^{p,+}\}$.

For the proof see Ukai and Asano[41].

We remark that, in order to prove this lemma and the two subsequent theorems, one needs a space of at least three dimensions; no analogous result is known for two-dimensional flows. This is related to the so-called "Stokes-paradox", which was discovered by Stokes for the Navier–Stokes equations and extended to the Boltzmann equation by Cercignani[21]. We shall discuss this in Chapter 6.

This lemma and Theorem 4.8.2 permit the evaluation of the right-hand side of Eq. (4.8.31). In addition, we need some estimates for $R_{\mathbf{v}}(\lambda)$ and must use the same arguments as in Theorems 3.4.3 and 3.4.4. Let us define $L_r^{p,s}(V)$ in the same way as in (4.8.22) with $\Re_x^3 \times \Re_{\boldsymbol{\xi}}^3$ replaced by $V = \Omega \times \Re_{\boldsymbol{\xi}}^3$, and set

$$X_r^p = L_{r-1/p}^{p,\infty} \cap L_r^{\infty,\infty}, \qquad Z^q = L^{2,2} \cap L^{q,2}. \tag{4.8.33}$$

One can prove the following

Theorem 4.8.4. *Let* $1 \le q \le 2 \le p \le \infty$, $r > 3/2$, $\theta \in [0, 1)$, $m = 0, 1$ *with*

$$q^{-1} - p^{-1} > (2 - m)/(3 + \theta) \quad , \quad p^{-1} < 1 - 2/(3 + \theta). \tag{4.8.34}$$

Also, let $\alpha \in [0, 1]$ *and* $\gamma = 1 + p^{-1} - q^{-1}$. *Also with* a_1, v_1, σ_1 *of Lemma* 4.8.3, *set* $\overline{\Sigma} = \Sigma(a_1, \sigma_1) \times S_1[v_1]$. *Then*

(i) *There is a constant* $C \ge 0$ *such that for any* $(\lambda, \mathbf{v}) \in \overline{\Sigma}$,

$$|\mathbf{v}|^{\theta\gamma} \parallel (\lambda I - B_{\mathbf{v}})^{-1} (I - P_{\mathbf{v}})^m (\nu_{\mathbf{v}} I)^\alpha h \parallel_{L_{r-1/p}^{p,\infty}} \le C(\parallel h \parallel_{X_r^p} + \parallel (\nu_{\mathbf{v}} I)^\alpha h \parallel_{Z^q}). \tag{4.8.35}$$

(ii) *Let* $\epsilon > 0$ *and* $\delta > \theta\gamma$. *Let* $h_{\mathbf{v}}$ *be such that*

$$h_{\mathbf{v}} \in L^\infty(S_1[v_1]; X_r^p) \cap B^0(S_1[c_1]; X_{r-\epsilon}^p), \quad (\nu_{\mathbf{v}} I)^\alpha h_{\mathbf{v}} \in B^0(S_1[c_1]; Z^q); \tag{4.8.36}$$

then

$$|\mathbf{v}|^{\theta\gamma} (\lambda I - B_{\mathbf{v}})^{-1} (I - P_{\mathbf{v}})^m (\nu_{\mathbf{v}} I)^\alpha h_{\mathbf{v}} \in B^0(\overline{\Sigma}; L_{r-\epsilon-1/p}^{p,\infty}). \tag{4.8.37}$$

If we compare this result with Theorem 4.8.2, the behavior of $(\lambda I - B_{\mathbf{v}})^{-1}$ near $v = 0$ is worse than that of $U_j(\lambda, \mathbf{v})$. Let $m = \alpha = 0$ and let $h \in X_r^p \cap Z^q$; then, for $v \in S_1[v_1]$ fixed, $(\lambda I - B_{\mathbf{v}})^{-1} h \in B^0(\Sigma(a_1, \sigma_1); L_{r-\epsilon-1/p}^{p,\infty})$ so that $B_{\mathbf{v}}^{-1} h \in L_{r-\epsilon-1/p}^{p,\infty}$ exists as a limit of $-(\lambda I - B_{\mathbf{v}})^{-1} h$ as $\lambda \to 0$.

Using this inverse, we can solve Eqs. (4.8.12–14) in the form

$$\phi_{\mathbf{v}} = R_{\mathbf{v}}(0) h_{\mathbf{v}} - B_{\mathbf{v}}^{-1} K_{\mathbf{v}} R_{\mathbf{v}}(0) h_{\mathbf{v}}, \tag{4.8.38}$$

and prove

Theorem 4.8.5. *Let* $p \in [2, \infty]$, $\theta \in [0, 1)$ *with*

$$p^{-1} < 1 - 2/(3 + \theta). \tag{4.8.39}$$

Let $r > 3$ *and assume that*

$$h_{\mathbf{v}} \in B^0(S_1[c_1]; Y_r^{\infty,-}), \quad \| h_{\mathbf{v}} \| = O(|\mathbf{v}|) \qquad (v \to 0). \tag{4.8.40}$$

Then $\phi_{\mathbf{v}}$ *solves* (4.8.12–14) *in* L^p*-sense and, with* $\gamma = 2 - 1/p$,

$$\phi_{\mathbf{v}} \in B^0(S_1[c_1]; L_r^{p,\infty}),$$

$$\| \phi_{\mathbf{v}} \| = O(|\mathbf{v}|^{1-\theta\gamma}) \qquad (v \to 0). \tag{4.8.41}$$

For the proof, we refer to the paper by Ukai and Asano[38].

We remark that the second condition in (4.8.40) is satisfied if, as it was assumed before,

$$|\beta - \beta_w| \leq \eta |\mathbf{v}| \qquad (\eta \geq 0). \tag{4.8.42}$$

In order to solve the nonlinear problem (4.8.12), we must now estimate $B_{\mathbf{v}}^{-1}\Gamma(g, h)$. This is done with the following

Lemma 4.8.6. *Let* $\theta \in (0, 1)$ *and* $r > 5/2$. *Assume that*

$$(3 + \theta)/(1 + \theta) < p < 3 + \theta \tag{4.8.43}$$

and let $\gamma = 1 + 2/p$. *There is a constant* $C \geq 0$ *such that, for* $v \in S_1[c_1]$,

$$\| B_{\mathbf{v}}^{-1}\Gamma(g, h) \| \leq C|\mathbf{v}|^{-\theta\gamma} \| g \| \| h \| \qquad \text{in } X^p{}_r. \tag{4.8.44}$$

For the proof we refer again to the paper by Ukai and Asano[41].

This lemma and Theorem 4.8.5 enable us to apply the contraction mapping technique to solve the steady problem in the form (4.8.12). At a first glance, however, (4.8.44) does not seem to be good enough, because, if we choose $\theta \neq 0$, it diverges as $v \to 0$, while the choice $\theta = 0$ is excluded in Lemma 4.8.6. The nice behavior of $\phi_{\mathbf{v}}$ indicated in (4.8.41), however, compensates for this defect of the estimate of $\| B_{\mathbf{v}}^{-1}\Gamma(g, h) \|$. We can find α such that

$$\alpha_1 \equiv \theta(1 + 2p^{-1}) < \alpha < 1 - \theta(2 - p^{-1}) \equiv \alpha_2. \tag{4.8.45}$$

Then one can prove the following

Theorem 4.8.7. *Let* $\theta \in [0, 2/7)$, $r > 5/2$, *and assume that* (4.8.43) *and* (4.8.45) *hold. Then there is a positive number* v_0 $(\leq v_1)$ *such that for any* $v \in S_1[v_0]$, *Eq.* (4.8.12) *has a unique solution* $h_{\mathbf{v}}$ *in* X_r^p *satisfying*

$$\| h_{\mathbf{v}} \|_{X_r^p} \leq C|\mathbf{v}|^{\alpha+\tau} \qquad (\alpha + \tau = \alpha_2 = 1 - \theta(2 - 1/p)). \tag{4.8.46}$$

For the proof see Ukai and Asano[41].

Before ending this section, we make a few remarks. First of all the continuity properties stated in Theorems 4.8.4 and 4.8.5 can be used to prove that

$$h_{\mathbf{v}} \in B^0(S_1[v_0]; X^p_{r-\epsilon}) \qquad (\epsilon > 0). \tag{4.8.47}$$

Also, it can be shown that $h_{\mathbf{v}} \in \hat{W}^p$ and satisfies Eq. (4.8.5) in L^p-sense.

We also explicitly remark that the exponent $\alpha_2 < 1$ in (4.8.46) is not quite satisfactory. In fact, heuristic considerations (see, e.g., Ref. 21) would suggest that the exponent should be unity (maybe with a different norm) so that the perturbation goes to zero linearly with $\mathbf{v}$. As a matter of fact, a more refined result was proved by Ukai and Asano[43] by using a more sophisticated technique (Nash's implicit function theorem) supplemented by decay estimates of $h_{\mathbf{v}}$ for large values of $|\mathbf{x}|$. According to this result, the solution in Theorem 4.8.7 satisfies (4.8.46) with $\alpha+\tau = 1$ ($\theta = 0$) in $L^{\infty,\infty}(\Omega\times\Re^3_{\boldsymbol{\xi}})\cap L^p_r(L^p(\Omega)\cap L^\infty(\Omega))$ $(1 < p < \infty,$ $r > 4)$.

4.9 Stability of the Steady Flow Past an Obstacle

We shall now deal with the unsteady flow of a gas past an obstacle $\mathcal{O}$ whose exterior will be again denoted by Ω. As in the previous section, at space infinity the distribution function will be a drifting Maxwellian $M_{\mathbf{v}}$. Then the distribution function f satisfies

$$\partial f/\partial t + \boldsymbol{\xi}\cdot\partial f/\partial\mathbf{x} = Q(f,f) \qquad \text{in } D, \tag{4.9.1}$$

$$\gamma_D^+ f(\mathbf{x},\boldsymbol{\xi},t) = K\gamma_D^- f \qquad \text{on } \partial D, \tag{4.9.2}$$

$$f(\mathbf{x},\boldsymbol{\xi},t) \to M_{\mathbf{v}}(\boldsymbol{\xi}) = \rho(2\pi/\beta)^{-3/2}\exp(-\beta|\boldsymbol{\xi}-\mathbf{v}|^2) \qquad (|\mathbf{x}|\to\infty), \tag{4.9.3}$$

$$f(\mathbf{x},\boldsymbol{\xi},0) = f_0(\mathbf{x},\boldsymbol{\xi}). \tag{4.9.4}$$

To solve this problem, following Ukai and Asano[42], we set

$$f = M_{\mathbf{v}} + M_w^{1/2}(h_{\mathbf{v}} + g) \tag{4.9.5}$$

where $h_{\mathbf{v}}$ is the steady solution, whose existence was discussed in the previous section. Eqs. (4.9.1–4) can be rewritten as follows:

$$\partial g/\partial t + \boldsymbol{\xi}\cdot\partial g/\partial\mathbf{x} = L_{\mathbf{v}}g + 2\Gamma(h_{\mathbf{v}},g) + \Gamma(g,g) \qquad \text{in } D, \tag{4.9.6}$$

$$\gamma_D^+ g(\mathbf{x},\boldsymbol{\xi},t) = \hat{K}\gamma_D^- g \qquad \text{on } \partial D, \tag{4.9.7}$$

$$g(\mathbf{x},\boldsymbol{\xi},t) \to 0 \qquad (|x|\to\infty), \tag{4.9.8}$$

$$f(\mathbf{x},\boldsymbol{\xi},0) = g_0(\mathbf{x},\boldsymbol{\xi}). \tag{4.9.9}$$

By definition, the steady solution $f_{\mathbf{v}}$ is asymptotically stable if (4.9.6–8) have a global solution g which tends to zero as $t \to \infty$, whenever g_o is sufficiently small. In order to prove the existence of such solution, we transform (4.9.6–8) into the following integral equation:

$$g(t) = E_{\mathbf{v}}(t)g_0 + \int_0^t E_{\mathbf{v}}(t-s)[2\Gamma(h_{\mathbf{v}}, g(s)) + \Gamma(g,g)(s)]ds \tag{4.9.10}$$

where $E_{\mathbf{v}}(t)$ denotes the semigroup generated by $B_{\mathbf{v}}$. In analogy with what we did in Chapter 3, we shall solve this equation by exploiting the decay properties of $E_{\mathbf{v}}(t)$. We remark that one might have used the linear operator $B_{\mathbf{v}} + 2\Gamma(h_{\mathbf{v}}, .)$ as a generator of a semigroup, thus giving Eq. (4.9.10) a simpler aspect; it seems hard, however, to obtain the decay properties of that semigroup.

Taking the inverse Laplace transform of (4.8.32) gives an explicit formula for $E_{\mathbf{v}}$:

$$E_{\mathbf{v}}(t) = \mathcal{R}E_{\mathbf{v}}^{\infty}(t)\mathcal{E} + (\gamma_D^{+}\mathcal{R}E_{\mathbf{v}}^{\infty\dagger}(t)\mathcal{E})^{\dagger} *_t D_{\mathbf{v}}(t) *_t \overline{K}E_{\mathbf{v}}^{\infty}\mathcal{E} \tag{4.9.11}$$

where $E_{\mathbf{v}}^{\infty}(t)$ clearly means the semigroup generated by $B_{\mathbf{v}}^{\infty}$, $*_t$ is the convolution in t and $D_{\mathbf{v}}(t)$ the inverse Laplace transform of $(I - T_{\mathbf{v}}(\lambda))^{-1}$, as defined in Chapter 3.

If we make use of Theorem 4.8.1 and proceed as in the proof of Theorem 3.4.3 we obtain

Theorem 4.9.1. *Let $1 \le q \le 2 \le p \le \infty$ and $m = 0, 1$. Then,*

$$\| E_{\mathbf{v}}^{\infty}(t)(I - P_{\mathbf{v}})^m h \|_{L_r^{p,\infty}} \le C(1+t)^{-\gamma - m/2} \| h \|_{L_r^{p,\infty} \cap Z^q} \tag{4.9.12}$$

with $\gamma = 3(p-q)/(2pq)$ and $C \ge 0$ independent of v, t, h.

By means of this theorem one can obtain[42] the following

Lemma 4.9.2. *Let v_1 be the same as in Lemma 4.8.3. Then, for each $\theta \in [0, 1)$, there is a constant $C \ge 0$ such that*

$$\| (D_{\mathbf{v}}(t) - I)h \|_{Y_r^{\infty,+}} \le C|\mathbf{v}|^{-\theta}(1+t)^{-\gamma} \| h \|_{Y_r^{\infty,+}} \tag{4.9.13}$$

holds for all $v \in S_1[v_1]$, with $\gamma = 1 + \theta/2$.

Theorem 4.9.1 and Lemma 4.9.2 are the estimates that we need to deal with Eq. (4.9.11).

We are now ready to deal with the existence theorem for Eq. (4.9.10), whose right-hand side we denote by $N(g)$. In order to evaluate the second (linear) term of $N(v)$, it is necessary to have $\gamma > 1$ in (4.9.12) ($m = 1$) and (4.9.13), while for the third (nonlinear) term, it suffices to have $\gamma > 1/2$. For the former, therefore, we should take $\theta > 0$ in (4.9.13) and a divergent factor $|\mathbf{v}|^{-\theta}$ appears, but this can be cancelled by means of (4.8.45). In any case, a careful choice of parameters is needed. Write p, θ of (4.8.43) as p_0, θ_0 and impose the additional condition $p_0 < 3$. Let α be as in (4.8.48) and let

$$p \in [2,4] \cap (3, (1/2 - 1/p_0)^{-1}),$$
$$q \in [1,2] \cap [1, (1/p + 1/3)^{-1}), \quad \theta \in (0, \alpha), \quad r > 5/2,$$
$$\gamma = \min\Big(3(p-q)/(2pq), (n/p_0 + 1)/2\Big). \tag{4.9.14}$$

Then $\gamma > 1/2$. Set

$$| \parallel g \parallel | = \sup_{t \geq 0} (1+t)^{\gamma} \parallel g \parallel_{X_r^p} . \tag{4.9.15}$$

We have

$$| \parallel N(g) \parallel | \leq C(\parallel g_0 \parallel_{L_r^{p,\infty} \cap Z^q} + (|\mathbf{v}|^{-\theta} a + | \parallel g \parallel |) | \parallel g \parallel |), \tag{4.9.16}$$

$$| \parallel N(g) - N(h) \parallel | \leq C((|\mathbf{v}|^{-\theta} a + | \parallel g \parallel | + | \parallel h \parallel |) | \parallel g - h \parallel |), \tag{4.9.17}$$

where $a = \parallel h_{\mathbf{v}} \parallel$ in $X_r^p, p = p_0$. By (4.9.52), $|\mathbf{v}|^{-\theta} a \to 0$ as $v \to 0$, so N is contractive if g_0 and v are sufficiently small. Thus we have proved the stability property stated in

Theorem 4.9.3. *Let us assume* (4.9.14)*. Then, there are positive constants* a_0, a_1, v_0 *such that for any* $v \in S_1(v_0)$ *and if* $\parallel g_0 \parallel \leq a_0$ *in* $X_r^p \cap Z^q$*, where* Z^q *was defined in* (4.8.33)*, Eq.* (4.9.10) *has a global solution*

$$g = g(t) \in B^0([0, \infty); X_r^p), \qquad \parallel g(t) \parallel \leq a_1 (1+t)^{-\gamma}.$$

4.10 Concluding Remarks

In this chapter we have dealt with existing results in the theory of existence and uniqueness for initial-boundary and pure boundary value problems for the Boltzmann equation. The most notable absence in this chapter concerns the existence of solutions far from equilibrium for pure boundary value problems and initial-boundary value problems for boundary data incompatible with a uniform Maxwellian solution. Concerning the first of these problems, for a long time there has been known a result in the case when the solution depends on just one space coordinate (say x) by Arkeryd, Cercignani and Illner[4], which had, however, a rather serious restriction, i.e., a cutoff in the small values of the x-velocity component; in addition the proof did not apply to hard sphere molecules but only to particles interacting with soft potentials. In the last ten years, important progress has been achieved thanks to the work of Arkerd and Nouri[5−11]. As for the initial-boundary value problems with general boundary data, the difficulties lie with large velocities; this was already clear from an argument used by Kawashima[30] for a one-dimensional discrete velocity model and is fully confirmed by a paper by Arkeryd and Cercignani[3]. One should also mention the work done by Maslova in this field; for this we refer to her survey[35].

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Chapter 5

Slow Flows in a Slab

5.1 Solving the Linearized Boltzmann Equation in a Slab

The mathematical theory of perturbations of equilibria presented in the previous chapters indicates that, if the deviation from a Maxwellian is very small, a very good approximation to the solution is provided by the linearized Boltzmann equation where the quadratic collision operator is replaced by the linearized collision operator, related to the bilinear operator defined in Eq. (1.4.3) by Eq. (3.1.4). In the applications one prefers to write the perturbed distribution function as $f = M(1+h)$ rather than $f = M + M^{1/2}h$ as was done in the previous chapter. Henceforth we adopt this convention and define

$$Lh = 2M^{-1}Q(Mh, M) \tag{5.1.1}$$

where M is a Maxwellian distribution, usually with zero bulk velocity. When we want to emphasize the fact that we linearize with respect to a given Maxwellian, we write L_M instead of just L.

A more explicit expression of Lh reads

$$Lh = \int_{\Re^3}\int_{\mathcal{B}_+} M_*(h' + h'_* - h_* - h)B(\theta, V)d\boldsymbol{\xi}_* d\mathbf{n} \tag{5.1.2}$$

where we have taken into account that $M'M'_* = MM_*$. Because of Eq. (5.4.10) (with Mh in place of f, M in place of g and g in place of ϕ), we have the identity

$$\int_{\Re^3} MgLhd\boldsymbol{\xi} = -\frac{1}{4}\int_{\Re^3}\int_{\Re^3}\int_{\mathcal{B}_+}(h' + h'_* - h - h_*)(g' + g'_* - g - g_*)B(\theta, V)d\boldsymbol{\xi}_* d\boldsymbol{\xi} d\mathbf{n}. \tag{5.1.3}$$

This relation expresses a basic property of the linearized collision term. In the new notation we must consider the scalar product in the Hilbert space of square summable functions of $\boldsymbol{\xi}$ endowed with a scalar product weighted with M:

$$(g, h) = \int_{\Re^3} \overline{g} h M d\boldsymbol{\xi} \tag{5.1.4}$$

where the bar denotes complex conjugation. Then Eq. (5.1.7) (with $\overline{g}$ in place of g) gives (thanks to the symmetry of the expression in the right-hand side of Eq. (5.1.3) with respect to the interchange $g \Leftrightarrow h$):

$$(g, Lh) = (Lg, h). \tag{5.1.5}$$

Further,

$$(h, Lh) \leq 0 \tag{5.1.6}$$

and the equality sign holds if and only if

$$h' + h'_* - h - h_* = 0, \tag{5.1.7}$$

i.e., if and only if h is a collision invariant.

Eqs. (5.1.5) and (5.1.6) indicate that the operator L is symmetric and nonpositive in the aforementioned Hilbert space.

In order to investigate the structure of the solutions of the linearized Boltzmann equation, we consider the simplest boundary value problem, the so-called plane Couette flow. Let us consider a monatomic rarefied gas with average density ρ_0, in motion between two parallel plates located at $x = 0$ and $x = L$, respectively (see Fig. 5.1). The upper plate moves with velocity V, whereas the lower one is at rest.

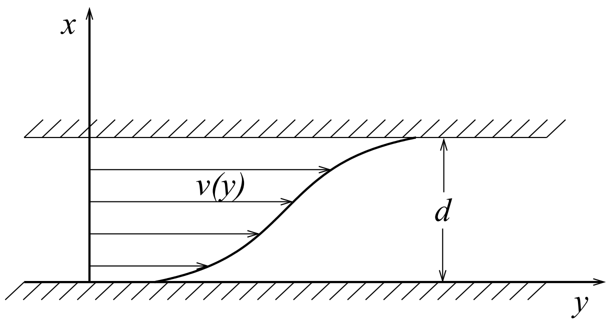

Figure 5.1: Geometry of a Couette flow.

In order to orient ourselves in a new field and chart the phenomena that can be expected, it is very useful to consider dimensional analysis, and give a look at the typical nondimensional parameters associated with the equations which rule these phenomena. Rarefied gas dynamics is no exception: it makes use of two basic nondimensional numbers, the so-called Knudsen number Kn_L based on the distance between the plates L ($\mathrm{Kn}_L = \lambda_0/L$) and the so-called speed ratio $S = U/V_{\mathrm{th}}$ (where $V_{\mathrm{th}} = (2RT_0)^{1/2}$ is the thermal speed and T_0 the temperature of the gas at $t = 0$), related to the Mach number Ma (the ratio between V and the speed of sound for a monatomic gas in continuum mechanics) by Ma$= (6/5)^{1/2}S = 1.095\,S$. λ_0 is the mean free path corresponding to the basic Maxwellian.

For steady solutions depending on just one space-coordinate x_1, the linearized Boltzmann equation can be rewritten as

$$\xi_1 \partial_x h = L_M h\,. \tag{5.1.8}$$

We shall assume, as is usually done with little loss of generality, that the bulk velocity in the Maxwellian is zero and we shall denote the unperturbed density and temperature by ρ_0 and T_0.

Although the equation is now linear, and hence all the weapons of linear analysis are available, it is far from easy to solve for a given boundary value problem, such as Couette flow. Yet it is possible to gain an insight on the behavior of the general solution of Eq. (5.1.8).

This solution can be found by looking for solutions of exponential form in x, familiar from the solution of ordinary differential equations

$$h_\gamma = g_\gamma(\boldsymbol{\xi}) \exp(\gamma x)\,. \tag{5.1.9}$$

Inserting this expression into Eq. (5.1.8), we find that the equation is satisfied, provided $g_\gamma(\boldsymbol{\xi})$ is a solution of

$$L_M g_\gamma = \gamma \xi_1 g_\gamma\,. \tag{5.1.10}$$

The study of this equation is not so simple; explicit solutions are available only if models, such as BGK, are used (see next chapter). It is possible however to study the set of values of γ for which Eq. (5.1.10) has a solution. The reader is invited to consult references 5–7 for details.

The first important result is that no complex values are admitted for γ. In addition the set of admitted values is symmetric with respect to the origin, and at least two cases may occur; either the set is made up of the two half-lines $\gamma \le -\overline{\gamma}$ and $\gamma \ge \overline{\gamma}$, where $\overline{\gamma}$ is some nonnegative number, plus discrete values between $-\overline{\gamma}$ and $\overline{\gamma}$, or it coincides with the entire real axis. The first case occurs for hard sphere molecules, the second for molecules interacting at a distance with an angular cutoff.

Among the possible values there is always $\gamma = 0$ (in the first of the two cases above, it may be the only discrete value between $-\overline{\gamma}$ and $\overline{\gamma}$). The case $\gamma = 0$ is special for two reasons: first, it leads to solutions that do not have an exponential behavior in x; second, the value $\gamma = 0$ is degenerate and offers some surprises. If we let $\gamma = 0$ in Eq. (5.1.5), we see that there are five possible solutions, the collision invariants; thus the eigenvalue $\gamma = 0$ is at least fivefold degenerate. It turns out that it is eightfold degenerate, but the additional degeneracy does not show up in terms of more functions satisfying Eq. (5.1.10). The situation is similar to the case of the ordinary differential equation $f'' = 0$. If we look for exponential solutions of the form $f = C\exp(\gamma x)$, for a nonzero constant $C = 0$, we obtain $\gamma^2 = 0$. In addition to $f = C$, we know that we have another, linearly independent, solution of the form $f = Dx$, where D is an arbitrary constant. In the same way, it turns out that, in order to obtain the general solution of Eq. (5.1.8), it is not enough to assume a linear combination of functions of the form (5.1.9); we must also add solutions which are linear in x. Thus we must look for this kind of solution. If we insert $h = A(\boldsymbol{\xi})x + B(\boldsymbol{\xi})$ in Eq. (5.1.8), we obtain, equating terms of zeroth and first degree in x:

$$\xi_1 A = L_M B \qquad 0 = L_M A\,. \tag{5.1.11}$$

Thus A must be a collision invariant ψ_α, but, in order for the equation for B to be solvable, $\int \xi_1 A\psi_\beta d\boldsymbol{\xi}$ must be zero for any collision invariant ψ_β ($\beta = 0, \ldots, 4$). This condition is automatically satisfied when either A or ψ_β do not contain a term proportional to ξ_1. When A is proportional to ξ_1, then the solvability condition is not satisfied (to see this, it is sufficient to let $\psi_\beta = 1$). On the other hand, if $\psi_\beta = \xi_1$, among the remaining collision invariants ψ_α, ψ_2 and ψ_3 satisfy the solvability condition, whereas ψ_0 does not and $\psi_4 = |\boldsymbol{\xi}|^2$ does not either; there is, however, a linear combination of ψ_0 and ψ_4 which satisfies the condition and hence, in the rest of this section, we let ψ_4 denote this linear combination, $\psi_4 = |\boldsymbol{\xi}|^2 - 5RT_0$. Then we have just three solutions linear in x (this justifies the previous statement that the eigenvalue $\gamma = 0$ is eightfold degenerate), and we can write the general solution of Eq. (5.1.8) in the following form:

$$\begin{aligned} h = \ & \sum_{\alpha=0}^{4} A_\alpha\psi_\alpha + \sum_{\alpha=2}^{4} B_\alpha[\psi_\alpha x + L^{-1}(\xi_1\psi_\alpha)] \\ & + \int_{-\infty}^{-\overline{\gamma}} C(\gamma)g_\gamma(\boldsymbol{\xi})\exp(\gamma x)d\gamma + \int_{\overline{\gamma}}^{\infty} C(\gamma)g_\gamma(\boldsymbol{\xi})\exp(\gamma x)d\gamma\,, \end{aligned} \tag{5.1.12}$$

where $\overline{\gamma}$ is nonnegative. In the case $\overline{\gamma} \neq 0$, there might be discrete exponential terms which we have omitted for simplicity. Further, since the solution of Eq. (5.1.10) is determined up to a constant factor depending upon γ, we have written the contribution as the product of a fixed factor $g_\gamma(\boldsymbol{\xi})$, normalized in some way, and an arbitrary weight $C(\gamma)$, which changes from one solution to another. This weight and, likewise, the coefficients A_α and B_α are determined by the boundary conditions. It can be shown (see Refs. 2 and 4) that Eq. (5.1.12) really provides the general solution of Eq. (5.1.8).

The above expression contains important information on the behavior of the solution. There are terms which have exponential behavior and terms which are polynomials of at most first degree in x.

Let us consider the exponential terms first. A feature that strikes the eye is that both increasing and decreasing exponentials are present; this may look odd, if one compares these terms with similar solutions in which time replaces the space variable x. In that case, in fact, the increasing exponentials are usually absent. A moment's thought will however show that this feature is absolutely required, because the increasing exponentials become decreasing, if we look at decreasing values of x. Thus, if we have two boundaries, located, say, at $x = 0$ and $x = L$, the terms with positive and negative values of γ will describe terms which decrease when moving away from the boundaries in the interval $[0, L]$. To see this in an explicit fashion, we exhibit a strikingly simple example, which embodies the essential features of Eq. (5.1.8) as far as the exponential terms are concerned. Let us consider the equation

$$\xi_1 \partial_x h + \nu h = 0\,, \tag{5.1.13}$$

where ν is a constant. The general solution is obviously

$$h = A(\xi_1) \exp(-\frac{\nu x}{\xi_1}) \tag{5.1.14}$$

where the constant of integration A depends on ξ_1 as well as on other parameters not explicitly appearing in Eq. (5.1.13), such as ξ_2 and ξ_3. If we assign the values of h at $x = 0$ for $\xi_1 > 0$, $h_+(\xi_1)$, and at $x = L$ for $\xi_1 < 0$, $h_-(\xi_1)$, we have the following solution:

$$h = h_+(\xi_1) \exp(-\frac{\nu x}{\xi_1}) \quad \text{for}\, \xi_1 > 0\,,$$

$$h = h_-(\xi_1) \exp(-\frac{\nu(L-x)}{|\xi_1|}) \quad \text{for}\, \xi_1 < 0\,, \tag{5.1.15}$$

where we have written $-|\xi_1|$ in place of ξ_1 when the latter is negative, in order to emphasize the signs in the exponentials. We see that the solution exhibits a decreasing exponential for $\xi_1 > 0$ and an increasing one for $\xi_1 < 0$. However, they are both bounded in x and one of them decreases away from one of the boundaries, $x = 0$ or $x = L$ respectively, in the interval $[0, L]$. The term that does not decrease is exponentially small, of order $\exp(-\nu L/|\xi_1|)$ near the corresponding boundary.

Thus the exponential terms play no role away from the boundaries, provided that the latter are sufficiently away from each other. How far away, we can see by remarking that γ has the dimensions of an inverse length; though γ takes infinitely many values, we can surmise that a typical magnitude of γ in a significant contribution to the solution will be of the order of the inverse of the mean free path. Thus, provided the boundaries are several mean free paths apart, the exponential terms will give a significant contribution just in thin layers near the boundaries (called the Knudsen layers).

Let us turn now to the other terms in Eq. (5.1.12). It is easy to compute the contributions of these terms to the first few moments of the distribution function. Here is the result, where the superscript F denotes that the contributions from the exponential terms do not appear (though the contribution from the unperturbed Maxwellian is present):

$$\rho^F = \rho_0[1 + A_0 - 2RT_0(A_4 + B_4 x)]\,,$$

$$\begin{aligned}
v_1^F &= A_1 R T_0 \,, \\
v_i^F &= A_i R T_0 + B_i R T_0 x \quad (i = 2,3) \,, \\
T^F &= T_0[1 + 2RT_0(A_4 + B_4 x)] \,, \\
p_{ij}^F &= RT_0\rho_0(1 + A_0)\delta_{ij} - \mu_0(B_i\delta_{1j} + B_j\delta_{1i})RT_0 \quad (i,j = 1,2,3) \quad (B_1 = 0) \,, \\
q_1^F &= -2\kappa_0 B_4 R T_0^2 \,, \\
q_i^F &= 0 \quad (i = 2,3) \,.
\end{aligned} \tag{5.1.16}$$

Here μ_0 and κ_0 are two functions of T_0 given by

$$\mu_0 = -(RT_0)^{-1} \int_{R^3} M c_1 c_2 L_M^{-1}(c_1 c_2) d\mathbf{c} \,,$$

$$\kappa_0 = -(4RT_0^2)^{-1} \int_{R^3} M c_1 |\mathbf{c}|^2 L_M^{-1}(c_1(|\mathbf{c}|^2 - 5RT_0)) d\mathbf{c} \tag{5.1.17}$$

where L_M^{-1} is the inverse of L_M in the subset of functions orthogonal to the collision invariants. We thus see that the stress tensor and the heat flow vector satisfy the Navier–Stokes and Fourier constitutive relations; further it is easy to see that ρ^F, $\mathbf{v}^F$ and T^F satisfy the Navier–Stokes–Fourier equations linearized about $\rho = \rho_0$, $\mathbf{v} = 0$ and $T = T_0$. The coefficients μ_0 and κ_0 have the meaning of viscosity and heat conductivity, respectively, evaluated at temperature T_0. In general, μ and κ will denote the same transport coefficients for a generic temperature T.

Thus we have the following picture: provided the plates are sufficiently far apart (several mean free paths), there are two Knudsen layers near the boundaries, where the behavior of the solution is strongly dependent on the boundary conditions, and a central core (a few mean free paths away from the plates), where the solution of the Navier–Stokes equations holds (with a slight reminiscence of the boundary conditions). If the plates are close in terms of the mean free path, then all the terms in the general solution are simultaneously important. If the mean free path is larger than the distance between the plates, the exponential terms will dominate.

Although we have given evidence for the above statements just in the case of the linearized Boltzmann equation, there is strong evidence that this qualitative picture applies to nonlinear flows as well, with a major exception. In general, compressible flows develop shock waves at large speeds and these do not appear in Eq. (5.1.12). These shocks are not surfaces of discontinuity as for an ideal fluid, governed by the Euler equations, but layers of rapid change of the solution (on the scale of the mean free path). One can obtain solutions for flows containing structured shocks from the Navier–Stokes equations, but, since they change significantly on the scale of the mean free path, they are inaccurate. Other regions where this picture is inaccurate are the zones of high rarefaction, where nearly free-molecular conditions may prevail, even if the rest of the flow is reasonably described in terms of Navier–Stokes equations, Knudsen layers and shock layers.

5.2 Model Equations

When trying to solve the Boltzmann equation for practical problems, one of the major shortcomings is the complicated structure of the collision term, Eq. (1.4.2). When one is not interested in fine details, it is possible to obtain reasonable results by replacing the collision integral by a so-called collision model, a simpler expression $J(f)$ which retains only the qualitative and average properties of the collision term $Q(f, f)$. The equation for the distribution function is then called a kinetic model or a model equation.

The most widely known collision model is usually called the Bhatnagar, Gross and Krook (BGK) model, although Welander proposed it independently at about the same time as the above mentioned authors[4,20]. It reads as follows:

$$J(f) = \nu[\Phi(\boldsymbol{\xi}) - f(\boldsymbol{\xi})] \tag{5.2.1}$$

where the collision frequency ν is independent of $\boldsymbol{\xi}$ (but depends on the density ρ and the temperature T) and Φ denotes the local Maxwellian, i.e., the (unique) Maxwellian having the same density, bulk velocity and temperature as f:

$$f = \rho(2\pi RT)^{-3/2}\exp[-|\boldsymbol{\xi} - \mathbf{v}|^2/(2RT)]. \tag{5.2.2}$$

Here $\rho, \mathbf{v}, T$ are chosen is such a way that for any collision invariant ψ we have

$$\int_{R^3} \psi(\boldsymbol{\xi})\Phi(\boldsymbol{\xi})d\boldsymbol{\xi} = \int_{R^3} \psi(\boldsymbol{\xi})f(\boldsymbol{\xi})d\boldsymbol{\xi}. \tag{5.2.3}$$

It is easily checked that, thanks to Eq. (5.2.3),

a) f and Φ have the same density, bulk velocity and temperature;

b) $J(f)$ satisfies conservation of mass, momentum and energy; i.e., for any collision invariant,
$$\int_{R^3} \psi(\boldsymbol{\xi})J(f)d\boldsymbol{\xi} = 0; \tag{5.2.4}$$

c) $J(f)$ satisfies the Boltzmann inequality
$$\int_{R^3} \log f J(f)d\boldsymbol{\xi} \leq 0, \tag{5.2.5}$$
the equality sign holding if and only if, f is a Maxwellian.

It should be remarked that the nonlinearity of the BGK collision model, Eq. (5.2.1), is much worse than the nonlinearity in $Q(f, f)$; in fact the latter is simply quadratic in f, while the former contains f in both the numerator and denominator of an exponential, because $\mathbf{v}$ and T are functionals of f, defined by Eqs. (1.6.2) and (1.6.27).

The main advantage in the use of the BGK model is that for any given problem one can deduce integral equations for $\rho, \mathbf{v}, T$, which can be solved with moderate effort on a computer. Another advantage of the BGK model is offered by its linearized form, as will become clear in the applications to be discussed in this book.

The BGK model has the same basic properties as the Boltzmann collision integral, but has some shortcomings. Some of them can be avoided by suitable modifications, at the expense, however, of the simplicity of the model. A first modification can be introduced in order to allow the collision frequency ν to depend on the molecular velocity, more precisely on the magnitude of the random velocity $\mathbf{c}$ (defined by Eq. (5.6.5)), while requiring that Eq. (5.2.4) still holds. All the basic properties, including Eq. (5.2.5), are retained, but the density, velocity and temperature appearing in Φ are not the local ones of the gas, but some fictitious local parameters related to five functionals of f different from $\rho, \mathbf{v}, T$; this follows from the fact that Eq. (5.2.3) must now be replaced by

$$\int_{R^3} \nu(|\mathbf{c}|)\psi(\boldsymbol{\xi})\Phi(\boldsymbol{\xi})d\boldsymbol{\xi} = \int_{R^3} \nu(|\mathbf{c}|)\psi(\boldsymbol{\xi})f(\boldsymbol{\xi})d\boldsymbol{\xi}. \qquad (5.2.6)$$

A different kind of correction to the BGK model is obtained when a complete agreement with the compressible Navier–Stokes equations is required for large values of the collision frequency. In fact the BGK model has only one parameter (at a fixed space point and time instant), i.e., the collision frequency ν; the latter can be adjusted to give a correct value for either the viscosity μ or the heat conductivity κ, but not for both. This is shown by the fact that the Prandtl number $\mathrm{Pr} = \mu/c_p\kappa$ (where c_p is the specific heat at constant pressure) turns out[5,6] to be unity for the BGK model, while it is about 2/3 for a monatomic gas (according to both experimental data and the Boltzmann equation). In order to have a correct value for the Prandtl number, one is led[14,15] to replacing the local Maxwellian in Eq. (5.2.1) by

$$\Phi(\boldsymbol{\xi}) = \rho(\pi)^{-3/2}(\det \mathsf{A})^{1/2} \exp\left(-(\boldsymbol{\xi} - \mathbf{v}) \cdot [\mathsf{A}(\boldsymbol{\xi} - \mathbf{v})]\right) \qquad (5.2.7)$$

where A is the inverse of the matrix

$$\mathsf{A}^{-1} = (2RT/\,\mathrm{Pr})\mathsf{I} - 2(1 - \mathrm{Pr})\mathsf{p}/(\rho\,\mathrm{Pr}) \qquad (5.2.8)$$

where I is the identity and p the stress matrix. If we let $\mathrm{Pr} = 1$, we recover the BGK model.

Only rather recently[3] this model (called ellipsoidal statistical (ES) model) has been shown to possess the property expressed by Eq. (5.2.5). Hence the H-theorem holds for the ES model.

Other models with different choices of Φ have been proposed[18,6] but they are not so interesting, except for linearized problems (see next section).

Another model is the integro-differential model proposed by Lebowitz, Frisch and Helfand[17], which is similar to the Fokker–Planck equation used in the theory of Brownian motion. This model reads as follows:

$$J(f) = D \sum_{k=1}^{3} \left[\frac{\partial^2 f}{\partial \xi_k^2} + \frac{1}{RT} \frac{\partial}{\partial \xi_k} [(\xi_k - v_k) f] \right] \tag{5.2.9}$$

where D is a function of the local density ρ and the local temperature T. If we take D proportional to the pressure $p = \rho RT$, Eq. (5.2.9) has the same kind of nonlinearity (*i.e.* quadratic) as the true Boltzmann equation.

5.3 Linearized Collision Models

In order to get further insight into the structure of the solutions of the Boltzmann equation, it is useful to adopt a simplified model, such as the BGK model, introduced in the previous section. The viscosity coefficient and the heat conductivity turn out to be simply related to the collision frequency and the Prandtl number turns out to be exactly unity, as opposed to the value 2/3, which is exact for Maxwell molecules and reasonably accurate for other molecular models. This shows a rather large error, of the order of 30%. Yet, frequently errors are smaller than this, especially when suitable tricks are used, such as the adjustment of the value of the collision frequency.

The main advantages of the use of models appear when one tries to solve the linearized Boltzmann equation and hence we shall briefly deal with the use of models for the linearized Boltzmann equation. If we consider the BGK model and linearize about a fixed Maxwellian distribution, M, we have essentially to approximate the local Maxwellian Φ appearing in Eq. (5.2.1) in terms of M and the moments of h. A simple calculation gives the following linearized operator:

$$\begin{aligned} L_{BGK} = \quad & \nu_0 \left[\int \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* + \frac{\boldsymbol{\xi}}{RT_0} \cdot \int \boldsymbol{\xi}_* \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* \right. \\ & \left. + \left(\frac{|\boldsymbol{\xi}|^2}{2RT_0} - \frac{3}{2}\right) \int \left(\frac{|\boldsymbol{\xi}_*|^2}{2RT_0} - \frac{3}{2}\right) \hat{M}(\boldsymbol{\xi}_*) h(\boldsymbol{\xi}_*) d\boldsymbol{\xi}_* - h \right] \end{aligned} \tag{5.3.1}$$

where ν_0 is the collision frequency evaluated at the density ρ_0 and temperature T_0 of the unperturbed state, and $\hat{M}$ denotes M/ρ_0. The operator (5.3.1) has a simple structure. It can be used to transform linearized problems into rather simple integral equations or systems of such equations. Another advantage is that sometimes the solutions can be computed explicitly, and their properties studied.

Further, the solution of problems in a slab or a half-space can be transformed to problems involving essentially the variable ξ_1 and not the entire vector $\boldsymbol{\xi}$[1,5]. To this end we remark that by momentum conservation $\int \xi_1 \hat{M} h d\boldsymbol{\xi}$ is a constant C. Then it is sufficient to write h in the following form:

$$\begin{aligned} h = \quad & h_0(x, \xi_1) + \frac{\xi_1 C}{RT_0} + \left(\frac{\xi_2^2 + \xi_3^2}{2RT_0} - 1 \right) h_1(x, \xi_1) \\ & + 2\xi_2 h_2(x, \xi_1) + 2\xi_3 h_3(x, \xi_1) + h_R(x, \boldsymbol{\xi}) \end{aligned} \tag{5.3.2}$$

where the decomposition is uniquely determined by the conditions

$$\int h_R \hat{M} d\boldsymbol{\xi} = 0\,, \quad \int \xi_i h_R \hat{M} d\boldsymbol{\xi} = 0 \ (i=2,3)\,, \quad \int \left(\frac{\xi_2^2+\xi_2^2}{2RT_0} - 1 \right) h_R \hat{M} d\boldsymbol{\xi} = 0. \tag{5.3.3}$$

Then the linearized BGK model is equivalent to the following five equations:

$$\begin{aligned}
\xi_1 \partial_x h_0 = \ & \nu_0 \left\{ \int \hat{M}_1(\xi_{1*}) h_0(\xi_{1*}) d\xi_{1*} + \frac{1}{6} (\frac{\xi_1^2}{RT_0} - 1) \right. \\
& \left. \times \left[\int (\frac{\xi_{1*}^2}{RT_0} - 1) \hat{M}_1(\xi_{1*}) h_0(\xi_{1*}) d\xi_{1*} + \int \hat{M}_1(\xi_{1*}) h_1(\xi_{1*}) d\xi_{1*} \right] - h_0 \right\}, \\
\xi_1 \partial_x h_1 = \ & \nu_0 \left\{ \frac{1}{3} (\frac{\xi_1^2}{RT_0} - 1) \left[\int \hat{M}_1(\xi_{1*}) h_0(\xi_{1*}) d\xi_{1*} \right. \right. , \\
& \left. \left. + \frac{2}{3} \int \hat{M}_1(\xi_{1*}) h_1(\xi_{1*}) d\xi_{1*} \right] - h_1] \right\}, \\
\xi_1 \partial_x h_i = \ & \nu_0 \left[\int \hat{M}_1(\xi_{1*}) h_i(\xi_{1*}) d\xi_{1*} - h_i \right] \quad (i = 2,3), \\
\xi_1 \partial_x h_R = \ & -\nu_0 h_R\,.
\end{aligned} \tag{5.3.4}$$

where $\hat{M}_1$ is the one-dimensional Maxwellian distribution obtained by integrating $\hat{M}$ with respect to ξ_2 and ξ_3.

The last equation in the above system is easy, but usually plays a little, if any, role. The previous relation contains two identical equations for $i = 2, 3$ and describe a shear flow when the plates move in the x_i direction. The first two equations are coupled and describe heat transfer problems (which are decoupled from motion in the linearized approximation).

The general solution of the above equations can be obtained in an explicit form[5,6]. In other words we can write the expansion (5.3.7) with an explicit expression for the eigensolution g_γ. Thus one can consider the problem of matching the boundary conditions. Here the half-range nature of the latter comes into play. If we equate the solution at each boundary to the data there, the resulting relations hold for either $\xi_1 > 0$ or $\xi_1 < 0$ and one cannot solve for the weights $C(\gamma)$ explicitly. One can obtain Fredholm equations determining $C(\gamma)$[8]. Actually, one can obtain two different equations, which lend themselves to obtaining converging expansions for either large or small values of the Knudsen number[8].

We recall here that other, more complicated models can be devised. Although they can be nonlinear, it is only at the linearized level that systematic approaches can be developed, without renouncing any property. The linearized models are essentially of two kinds. The first procedure relies on the use of the eigenfunctions of the linearized collision operator for Maxwell molecules, i.e., polynomials $\psi_\alpha(\boldsymbol{\xi})$ which are orthogonal with respect to a Maxwellian weight; in other words,

$(\psi_\alpha, \psi_\beta) = \delta_{\alpha\beta}$, where

$$(g, h) = \int ghMd\boldsymbol{\xi}. \tag{5.3.5}$$

Then we can obtain models of the form

$$L_N = \sum_{\alpha=0}^{N} \nu_\alpha \psi_\alpha(\psi_\alpha, h) - \nu_N h \tag{5.3.6}$$

where $\nu_\alpha = \nu_N$ for $\alpha = 0, 1, 2, 3, 4$. This model generalizes the BGK model (to which it reduces for $N = 4$) in a simple way and is capable of approximating the linearized collision operator for Maxwell molecules. A further generalization along the same lines is

$$L_N = \sum_{\alpha,\beta=0}^{N} \nu_{\alpha\beta} \psi_\alpha(\psi_\beta, h) - \nu_N h. \tag{5.3.7}$$

This model can approximate molecules other than Maxwell's, but some features are lost, especially at large speeds. This remark leads to considering other models having the form

$$L_N = \nu(|\boldsymbol{\xi}|) \left(\sum_{\alpha=0}^{N} \mu_\alpha \phi_\alpha(\nu\phi_\beta, h) - h \right), \tag{5.3.8}$$

where $\phi_\alpha(\boldsymbol{\xi})$ are suitable functions orthogonal with respect to a weight given by a Maxwellian distribution multiplied by a function $\nu = \nu(|\boldsymbol{\xi}|)$, the collision frequency $((\phi_\alpha, \nu\phi_\beta) = \delta_{\alpha\beta})$.

These models can be treated in the same way as the BGK model. Of course, the calculations become more complicated, but the qualitative features are the same. We shall not enter into details here and refer the reader to the literature[5,6].

5.4 Transformation of Models into Pure Integral Equations

One of the advantages of the models is that they can be transformed into pure integral equations. In this section we shall just consider the case of isothermal Couette flow to which we can apply the relevant equation of the system (5.3.4). We rewrite the latter abolishing all the subscripts, since no confusion arises:

$$\xi \partial_x h = \nu_0 [v(x) - h] . \tag{5.4.1}$$

Here we have replaced the integral by $v(x)$, the component of the bulk velocity along the y-axis, because this is the meaning of that integral. We want to solve the above equation with the following boundary conditions:

$$h = 0 \quad \text{for } x = 0 \text{ and } \xi > 0\,, \qquad h = V \quad \text{for } x = L \text{ and } \xi < 0\,. \tag{5.4.2}$$

Now we take advantage of the fact that the term $v(x)$ in Eq. (5.4.1) is independent of ξ and assume for a moment that it is known. Then we can write the solution of Eq. (5.4.1) with the boundary condition (5.4.2) as follows:

$$h = \frac{\nu_0}{\xi}\int_0^x v(x_*)\exp\left(-\nu_0\frac{x-x_*}{\xi}\right)dx_* \text{ for } \xi > 0$$

$$h = V\exp\left(-\nu_0\frac{L-x}{|\xi|}\right)+\frac{\nu_0}{|\xi|}\int_x^L v(x_*)\exp\left(-\nu_0\frac{|x-x_*|}{|\xi|}\right)dx_* \text{ for } \xi < 0. \quad (5.4.3)$$

This equation shows that h is known (at least in principle, since we must perform two integrations) when $v(x)$ is known. We must now obtain an equation for $v(x)$. To this end we take into account the fact that $v(x)$ is given by the integral appearing in Eq. (5.4.1). Then if we insert h as given by Eq. (5.4.3) into the latter integral, and equate the result to $v(x)$, we obtain the equation determining the latter quantity. The result reads as follows:

$$v(x) = \pi^{-1/2}VT_0\left(\frac{L-x}{\lambda}\right)+(\lambda)^{-1}\pi^{-1/2}\int_0^L T_{-1}\left(\frac{|x-x_*|}{\lambda}\right)v(x_*)dx_* \quad (5.4.4)$$

where we have introduced the so-called Abramowitz functions[1,2]:

$$T_n(s) = \int_0^\infty t^n\exp(-t^2-\frac{s}{t})dt \qquad (n = \cdots -1, 0, 1, 2, \dots)$$

such that $T_{n-1} = -dT_n/ds$ and $\lambda = (2RT_0)^{1/2}/\nu_0$ is a precise definition of the mean free path introduced in Eq. (1.2.4) can be solved by iteration, since the integral operator is contracting. This is, however, not the best method to solve the above integral equation. Discrete ordinate methods work very well. The general form of a numerical scheme is

$$v_j = S_j + \sum_k \alpha_{jk}v_k \quad (5.4.5)$$

where two possible choices for the source term S_j and the coefficients are[12]:

$$S_j = \pi^{-1/2}VT_0\left(\frac{L-\frac{2j-n+1}{2n}L}{\lambda}\right),$$

$$\alpha_{jk} = (\lambda)^{-1}\pi^{-1/2}\int_{\frac{2k-n}{2n}L}^{\frac{2k-n+2}{2n}L} T_{-1}\left(\frac{|\frac{2j-n+1}{2n}L-x_*|}{\lambda}\right)dx_*, \quad (5.4.6)$$

$$S_j = n\pi^{-1/2}V\int_{\frac{2j-n}{2n}L}^{\frac{2j-n+2}{2n}L} T_0\left(\frac{L-x}{\lambda}\right)dx,$$

$$\alpha_{jk} = n(2\lambda)^{-1}\pi^{-1/2}\int_{\frac{2j-n}{2n}L}^{\frac{2j-n+2}{2n}L}\int_{\frac{2k-n}{2n}L}^{\frac{2k-n+2}{2n}L} T_{-1}\left(\frac{|x-x_*|}{\lambda}\right)dxdx_*\,. \quad (5.4.7)$$

The integrals appearing here can be explicitly evaluated in terms of the functions T_0 and T_1.

As for the system of the first two equations of the system (5.3.4), it is possible, by an analogous procedure, to obtain a system of two integral equations for the perturbations of density and temperature.

Systems of integral equations (of increasing order) can be obtained[1] for the more general models considered at the end of the previous section.

The method of using integral equations was pioneered by Welander[20] for half-space problems and by Willis[21] in the case of a slab. Two schemes of the kind reported above were used by Cercignani and Daneri[12] to study plane Poiseuille flow (see Section 4) in 1963. The method of solving numerically the integral equations can be extended to nonlinear problems and was used for several years as the only method which could give reasonably accurate solutions on a computer[10–12]. It is still used to provide solutions with an accuracy that can, in principle, be made as high as one likes in both linearized and nonlinear problems.

5.5 Variational Methods

The integral equation approach lends itself to a variational solution. The main idea of this method (for linear problems) is the following. Suppose that we must solve the equation

$$\mathcal{L}h = S \tag{5.5.1}$$

where h is the unknown, $\mathcal{L}$ a linear operator and S a source term. Assume that we can form a bilinear expression $((g, h))$ such that $((\mathcal{L}g, h)) = ((g, \mathcal{L}h))$, for any pair $\{g, h\}$ in the set where we look for a solution. Then the expression (functional)

$$J(\tilde{h}) = ((\tilde{h}, \mathcal{L}\tilde{h})) - 2((S, \tilde{h})) \tag{5.5.2}$$

has the property that if we set $\tilde{h} = h + \eta$, then the terms of first degree in η disappear and $J(\tilde{h})$ reduces to $J(h) + ((\eta, \mathcal{L}\eta))$ if and only if h is a solution of Eq. (5.5.1). In other words if η is regarded as small (an error), $J(\tilde{h}) - J(h)$ becomes small of second order in the neighborhood of h, if and only if h is a solution of Eq. (5.5.1). Then we say that the solutions of the latter equation satisfy a variational principle, or make the functional in Eq. (5.5.2) stationary. Thus a way to look for solutions of Eq. (5.5.1) is to look for solutions which make the functional in Eq. (5.5.2) stationary (variational method).

The method is particularly useful if we know that $((\eta, \mathcal{L}\eta))$ is nonnegative (or nonpositive) because we can then characterize the solutions of Eq. (5.5.1) as maxima or minima of the functional (5.5.2). But, even if this is not the case, the property is useful. First of all, it gives a non-arbitrary recipe to select among approximations to the solution in a given class. Second, if we find that the functional J is related to some physical quantity, we can compute this quantity with high accuracy, even if we have a poor approximation to h. If the error η is of order

10%, then J will be in fact computed with an error of the order of 1%, because the deviation of $J(\tilde{h})$ from $J(h)$ is of order η^2, as we have seen.

The integral formulation of the models lends itself to application of the variational method[13]. Thus in the case of Eq. (5.4.4) the bilinear expression $((w,v))$ is simply $\int_0^L w(x)v(x)dx$ and the calculations are easy (see below). Further, the functional is related to the stress component p_{12} which is constant and gives the drag exerted by the gas on each plate. Thus this quantity can be computed with high accuracy (see below).

This method can be generalized to other problems and to the more complicated models discussed in the previous section[5]. It can also be used to obtain accurate finite ordinate schemes, by approximating the unknowns by trial functions which are piecewise constant. The second scheme in the previous section was obtained in this way[12].

In the case of the steady linearized Boltzmann equation, Eq. (5.1.8), a similar method can be used. Let us indicate by Dh the differential part appearing in the left-hand side (for the sake of generality we set $Dh = \boldsymbol{\xi}\cdot\partial_{\mathbf{x}}h$ in order to include problems with a more complicated geometry) and assume that there is a source term as well (we shall see an example of a source in Section 6) and write our equation in the form

$$Dh - Lh = S. \tag{5.5.3}$$

If we try the simplest possible bilinear expression,

$$((g,h)) = \int_0^L \int_{\Re^3} g(\mathbf{x},\boldsymbol{\xi})h(\mathbf{x},\boldsymbol{\xi})M d\mathbf{x}d\boldsymbol{\xi}, \tag{5.5.4}$$

and we use it with $\mathcal{L}h = Dh - Lh$, we cannot reproduce the symmetry property $((\mathcal{L}g,h)) = ((g,\mathcal{L}h))$. It works for Lh but not for Dh. There is however a trick[9] which leads to the desired result.

Let us introduce the parity operator in velocity space, P, such that $P[h(\boldsymbol{\xi})] = h(-\boldsymbol{\xi})$. Then we can think of replacing Eq (5.5.3) by

$$PDh - PLh = PS \tag{5.5.5}$$

because this is completely equivalent to the original equation. In addition, because of the central symmetry of the molecular interaction $PLh = LPh$, and the fact that we had no problems with L, is not destroyed by the fact that we use P. On the other hand we have by a partial integration:

$$((g,PDh)) = ((PDg,h)) + ((g^+,Ph^-))_B - ((Pg^-,h^+))_B. \tag{5.5.6}$$

Here $g^{\pm}$ denote the restrictions of a function defined on the boundary to positive, respectively negative, values of $\boldsymbol{\xi}\cdot\mathbf{n}$, where $\mathbf{n}$ is the unit vector normal to the boundary. In addition, we have put

$$((g^{\pm},h^{\pm}))_B = \int_{\partial\Omega}\int_{\pm\xi\cdot\mathbf{n}>0} |\boldsymbol{\xi}\cdot\mathbf{n}| g(\mathbf{x},\boldsymbol{\xi})h(\mathbf{x},\boldsymbol{\xi})M d\boldsymbol{\xi}d\sigma. \tag{5.5.7}$$

In the one-dimensional case, the integration over the boundary $\partial\Omega$ reduces to the sum of the boundary terms at $x = 0$ and $x = L$.

Clearly the last two terms in Eq. (5.5.6) do not fit in our description. We have two ways out of the difficulty. We first recall a property of the boundary conditions, discussed in Section 3.1. The boundary conditions must be linearized about the Maxwellian distribution M and this gives them the following form (see below):

$$h^+ = h_0 + Kh^-. \tag{5.5.8}$$

Because of reciprocity (Eq. (3.1.12)), we have

$$((Pg^-, Kh^-))_B = ((Kg^-, Ph^-))_B. \tag{5.5.9}$$

Hence, if we assume that both g and h satisfy the boundary conditions, we have

$$\begin{aligned}
&((g^+, Ph^-))_B - ((Pg^-, h^+))_B \\
&= ((h_0, Ph^-))_B - ((Pg^-, h_0))_B + ((Kg^-, Ph^-))_B - ((Pg^-, Kh^-))_B \\
&= ((h_0, Ph^-))_B - ((Pg^-, h_0))_B.
\end{aligned} \tag{5.5.10}$$

We remark that we can modify the solution of the problem by adding a combination of the collision invariants with constant coefficients. This does not modify the Boltzmann equation but can be used to modify the boundary conditions. Usually it is possible to dispose of the constant coefficients to make $((h_0, Ph^-))_B = 0$ (and, at the same time, of course, $((h_0, Pg^-))_B = 0$). We assume that this is the case. Using this relation and Eq. (5.5.9), Eq. (5.5.10) reduces to

$$((g^+, Ph^-))_B - ((Pg^-, h^+))_B = 0 \tag{5.5.11}$$

and the variational principle holds with the operator $\mathcal{L}h = PDh - PLh$ and the source PS.

This variational principle is correct but not so useful, because it can be used only with approximations which exactly satisfy the boundary conditions and it can be complicated to construct these approximations. Thus we follow another procedure by incorporating the boundary conditions in the functional. It is enough to consider

$$J(\tilde{h}) = ((\tilde{h}, PD\tilde{h} - PL\tilde{h})) - 2((PS, \tilde{h})) + ((P\tilde{h}^-, \tilde{h}^+ - K\tilde{h}^- - 2h_0))_B. \tag{5.5.12}$$

In fact, if we let $\tilde{h} = h + \eta$, we find that the terms linear in η disappear from J and the variational principle holds.

In agreement with what we said before, it is interesting to look at the value attained by J when $\tilde{h} = h$. Eq. (5.5.12) becomes

$$J(h) = -((PS, h)) - ((Ph^-, h_0))_B. \tag{5.5.13}$$

This result acquires its full meaning only when we examine the expressions for h_0 and S. In general $S = 0$ (for an important case in which this is not true, see

Section 12). If we let $S = 0$, then we must look at the expression of h_0. The boundary source has a special form because it arises from the linearization, about a Maxwellian distribution M, of a boundary condition of the form

$$f_+ = K_w f_-, \tag{5.5.14}$$

where K_w is an operator which has several properties, including

$$M_{w+} = K_w M_{w-}. \tag{5.5.15}$$

Now, if we let $f = M(1+h)$ in Eq. (5.5.14), we have

$$h_+ = \frac{K_w M_- h_-}{M_+} + \frac{K_w M_-}{M_+} - 1. \tag{5.5.16}$$

This relation is exact. We can now proceed to neglect terms of order higher than first in the perturbation parameters. We can replace in K_w the temperature and velocity of the wall by those of the Maxwellian M (i.e., T_0 and 0) and obtain a slightly different operator K_0. Thus we obtain the operator K, which we used before, by letting $K_0 M_- h_- / M_+ = K h_-$. Concerning the source, we have, using Eq. (5.5.15),

$$h_0 = \frac{K_w M_-}{M_+} - 1 = \frac{K_w M_-}{M_+} - \frac{K_w M_{w-}}{M_{w+}}.$$

Since M_w and M differ by terms of first order, we can replace K_w by K_0 because their difference is also of first order and would produce a term of second order in the expression of h_0:

$$h_0 = \frac{K_0 M_-}{M_+} - \frac{K_0 M_{w-}}{M_{w+}} = 1 - \frac{K_0 M_{w-}}{M_{w+}}. \tag{5.5.17}$$

Now,if we neglect terms of higher than first order in the speed of the wall and the temperature difference $T_w - T_0$, we have $M_w = M(1+\psi)$, where (recalling that M_w is determined up to the density that we can choose to be the same as in M) ψ can be explicitly computed to give

$$\psi = \frac{\boldsymbol{\xi} \cdot \mathbf{v}_w}{RT_0} + \left(\frac{|\boldsymbol{\xi}|}{2RT_0} - \frac{3}{2} \right) \frac{T_w - T_0}{T_0} \tag{5.5.18}$$

and, finally, neglecting again terms of order higher than first,

$$h_0 = \psi_+ - K\psi_-. \tag{5.5.19}$$

Then Eq. (5.5.13) with $S = 0$ gives

$$\begin{aligned} J(h) &= -((Ph^-, \psi_+))_B + ((Ph^-, K\psi_-))_B \\ &= -((Ph^-, \psi_+))_B + ((Kh^-, P\psi_-))_B \\ &= -((Ph^-, \psi_+))_B + ((h^+ - \psi^+ + K\psi^-, P\psi_-))_B \\ &= -((Ph^-, \psi_+))_B + ((h^+ -, P\psi_-))_B + ((K\psi^- - \psi^+, P\psi_-))_B. \end{aligned} \tag{5.5.20}$$

The last term is a known quantity, whereas the first and the second can be combined to given unknown quantities of physical importance. In fact, if we take into account the expression of ψ (Eq. (5.5.18)), we obtain

$$\begin{aligned}
&-((Ph^-,\psi_+))_B + ((h^+-,P\psi_-))_B \\
&= -\int \frac{\boldsymbol{\xi}\cdot\mathbf{v}_w}{RT_0}\boldsymbol{\xi}\cdot\mathbf{n}h(\mathbf{x},\boldsymbol{\xi})Md\boldsymbol{\xi}d\sigma + \int\left(\frac{|\boldsymbol{\xi}|^2}{2RT_0}-\frac{3}{2}\right)\frac{T_w-T_0}{T_0}\boldsymbol{\xi}\cdot\mathbf{n}h(\mathbf{x},\boldsymbol{\xi})Md\boldsymbol{\xi}d\sigma \\
&= -\frac{1}{RT_0}\left(\int \mathbf{p_n}\cdot\mathbf{v}_w d\sigma + \int q_{\mathbf{n}}\frac{T_w-T_0}{T_0}d\sigma\right).
\end{aligned} \tag{5.5.21}$$

Here $\mathbf{p_n}$ is the normal stress vector and $q_{\mathbf{n}}$ the normal component of the heat flow. The fact that the mass flow vanishes at the wall has been taken into account.

Because of the linearity of the problem, it is possible and convenient, without loss of generality, to consider separately the two cases $\mathbf{v}_w = 0$ and $T_w = T_0$. Then the two terms in the expression above occur in two different problems. For some typical problems $\mathbf{v}_w$ vanishes on just one part of the boundary, whereas it is a constant on the remaining part of the latter; then the factor multiplying this constant is the drag on the corresponding part of the boundary. Similarly one can consider the case in which the factor in front of q_n and relate the value of the functional to the heat transfer.

The two variational principles which have been discussed are related to each other[5].

To give a simple example of the use of the variational method method in kinetic theory, let us consider the case of Couette flow for the integral formulation of the BGK model, Eq. (5.4.4). The functional to be considered is

$$\begin{aligned}
J(\tilde{v}) = &\int_0^L [\tilde{v}(x)]^2 - \pi^{-1/2}(\lambda)^{-1}\int_0^L\int_0^L \tilde{v}(x)T_{-1}\left(\frac{|x-x_*|}{\lambda}\right)\tilde{v}(x_*)dxdx_* \\
&-2\pi^{-1/2}V\int_0^L \tilde{v(x)}T_0\left(\frac{L-x}{\lambda}\right)dx.
\end{aligned} \tag{5.5.22}$$

We remark that

$$J(v) = -\pi^{-1/2}V\int_0^L v(x)T_0\left(\frac{L-x}{\lambda}\right)dx. \tag{5.5.23}$$

Let us now consider the expression of the stress component p_{12}. In order to compute it, we have to integrate the expressions of h in (5.4.1) after multiplication by ξ, to obtain

$$\begin{aligned}
p_{12} = &(2RT_0)^{1/2}VT_1\left(\frac{L-x}{\lambda}\right) \\
&-(2RT_0)^{1/2}(\lambda)^{-1}\int_0^L T_0\left(\frac{|x-x_*|}{\lambda}\right)\operatorname{sgn}(x-x_*)v(x_*)dx_*.
\end{aligned} \tag{5.5.24}$$

We note that, as we know, p_{12} is constant. To check it, we can differentiate Eq. (5.5.24) with respect to x and use the fact that v satisfies Eq. (5.4.4) (the elementary property of the Abramowitz functions, $dT_n/ds = -T_{n-1}$ must also be used). Thus we can evaluate p_{12} for any value of x. If we choose $x = L$ and compare with Eq. (5.5.23), we obtain (using $T_1(0) = 1/2$)

$$p_{12} = \left(\frac{RT_0}{2}\right)^{1/2} V + \left(\frac{2RT_0}{V\pi}\right)^{1/2} (\lambda)^{-1} J(v). \tag{5.5.25}$$

Thus the stress has a direct relation to the stationary value (in this case a minimum) of the functional J and we can hope for an accurate expression of p_{12} by taking a rough approximation for v. The simplest choice is $\tilde{v} = V/2 + A(x - L/2)$ where A is a constant to be chosen in such a way as make the derivative of $J(Ax)$ with respect to A vanish. The reason why we choose the above form for the trial function rather than the simpler Ax is that there is a symmetry about the midpoint between the plates (in the linearized case). We know that a linear trial function is a very poor approximation to the true velocity profile, since it neglects the Knudsen layers completely. Yet, and this is the main advantage of the variational method, we shall obtain very accurate results for the stress tensor.

After some easy manipulations based on the properties of the T_n functions, we find[13] the following expression for $J(V/2 + A(x - L/2))$:

$$\begin{aligned}
&J(V/2 + A(x - L/2)) \\
&= A^2\pi^{-1/2}\left\{\frac{L^2}{2\lambda^2}\left[\frac{1}{2} + T_1\left(\frac{L}{\lambda}\right)\right] + 2\frac{L}{\lambda}T_2\left(\frac{L}{\lambda}\right) - \left[1 - T_3\left(\frac{L}{\lambda}\right)\right]\right\} \\
&\quad -(2\pi RT_0)^{-1/2}VA\left\{\frac{L}{\lambda}\left[2T_1\left(\frac{L}{\lambda}\right) + 1\right] + \left[2T_2\left(\frac{L}{\lambda}\right) - \frac{\pi^{1/2}}{2}\right]\right\}.
\end{aligned} \tag{5.5.26}$$

The minimum condition gives the value of A_0:

$$A_0 = \frac{(2RT_0)^{-1/2}V\left\{(L/\lambda)\left[2T_1(L/\lambda) + 1\right] + \left[2T_2(L/\lambda) - \frac{1}{2}\pi^{1/2}\right]\right\}}{\left\{(L/\lambda)^2\left[\frac{1}{2} + T_1(L/\lambda)\right] + 4L/\lambda T_2(L/\lambda) - 2\left[1 - T_3(L/\lambda)\right]\right\}}. \tag{5.5.27}$$

If we insert this into $J(V/2 + A_0(x - L/2))$ we can compute an approximate expression for p_{12} given by

$$p_{12} = \rho_0(2RT_0)^{1/2}VT_1(0) + \rho_0\left(\frac{2RT_0}{V\pi}\right)^{1/2}(\lambda)^{-1}J(V/2 + A_0(x - L/2)). \tag{5.5.28}$$

δ	Willis	Linear	Cubic
20.0	0.0807	0.0805	0.0805
10.0	0.1474	0.1474	0.1474
7.00	0.1964	0.1964	0.1963
5.00	0.2526	0.2524	0.2523
4.00	0.2946	0.2945	0.2943
3.00	0.3539	0.3537	0.3535
2.50	0.3938	0.3935	0.3933
2.00	0.4440	0.4438	0.4437
1.75	0.4745	0.4743	0.4742
1.50	0.5099	0.5097	0.5096
1.25	0.5517	0.5512	0.5511
1.00	0.6008	0.6008	0.6008
0.10	0.9258	0.9258	0.9258

Table 5.1. Comparison between the variational[13] and numerical[21] results for the nondimensional stress in plane Couette flow as a function of the inverse Knudsen number δ. The results with the variational method are computed with both a linear (third column) and a cubic trial function (fourth column).

We use the inverse Knudsen number $\delta = L/\lambda$ as an independent variable and put p_{12} in a nondimensional form π_{12} by dividing by its free-molecular value $p_{12}^{f.m.} = -\rho_0 V(RT_0/2\pi)^{1/2}$. The resulting values are tabulated versus δ in Table 5.1 (third column) and compared with the results obtained by Willis[21] through a numerical solution. The agreement is excellent, the difference being at most $5 \cdot 10^{-4}$. We can say something more, namely that the results obtained by the variational method are more accurate than Willis's, with one possible exception. As a matter of fact, the variational method gives for π_{12} a value approximated from above, and the values in the third column are, with the exception of the first row, never larger than the corresponding ones in the second column.

In order to check the accuracy of the method, we can use a cubic trial function $v = V/2 + A(x - L/2) + B(x - L/2)^3$. In this case the algebra is more formidable but still straightforward[13]. It is clear that the resulting values for π_{12} are only slightly different, the difference between the third and the fourth column being at most $2 \cdot 10^{-4}$. This confirms the accuracy of the method and the fact that the error in both the variational and Willis's results are less than 10^{-3}, the variational ones being slightly more accurate.

Let us now look at the application of the variational method to the linearized Boltzmann equation in its integro-differential formulation. Here the main difficulty lies in choosing the trial function. In fact the method based on the integral equation has a hidden advantage: no matter how bad is the trial function, we obtain the correct free-molecular limit, because the free streaming is already built in the method. That is why we could obtain such good results with a very simple trial function; the reason was that it was correct in the continuum regime and thus the variational method optimized the interpolation between the two extreme behaviors.

Now we need at least three constants to reproduce the limiting behaviors in a reasonable way and thus (following Ref. 9) we try:

$$\tilde{h} = 2\xi_3(\alpha x + \beta\xi_1 + \gamma \operatorname{sgn}\xi_1) \tag{5.5.29}$$

where α, β and γ are three adjustable constants. The advantages with respect to the previous method are that the calculations are easier (in the case of the BGK model) and that a simple rational approximation to π_{12} is obtained for any molecular model:

$$\pi_{12} = \frac{a + \pi^{1/2}\delta}{a + b\delta + c\delta^2}. \tag{5.5.30}$$

The constants a, b, c can be computed, in principle, for any molecular model. In order to make the definition of δ unequivocal, we let $\delta = L/\lambda$, where $\lambda = (\mu_0/p_0)(2RT_0)^{1/2}$ (this definition agrees with the previous one in the case of the BGK model. Then $c = 1$. Three cases were considered in Ref. 14, the BGK model), Maxwell molecules and hard spheres, with the following results:

$$a = \frac{4-\pi}{\pi-2} \cong 0.7519, \quad b = \frac{\pi^{3/2}}{2(\pi-2)} \cong 2.4388 \quad \text{(BGK)},$$

$$a = 0.2225, \quad b = 2.1400 \quad \text{(Maxwell molecules)},$$

$$a = 0.3264, \quad b = 2.1422 \quad \text{(hard spheres)}. \tag{5.5.31}$$

The maximum disagreement between the values of the stress for the BGK model and Willis's result is 0.5%. The results for Maxwell molecules and the BGK model are very close to each other except for high values of the Knudsen number ($\delta < 2$), where a difference of order 3% arises. Surprisingly enough, the results for hard spheres are, in this range, much closer than those for Maxwell molecules to those for the BGK model.

δ	Willis	BGK	Maxwell	hard spheres	hard spheres$_*$
20	0.0807	0.0805	0.0805	0.0801	0.0807
10	0.1474	0.1476	0.1476	0.1462	0.1483
7	0.1964	0.1969	0.1967	0.1943	0.1980
5	0.2526	0.2534	0.2529	0.2491	0.2550
4	0.2946	0.2958	0.2951	0.2900	0.2980
3	0.3539	0.3556	0.3542	0.3472	0.3583
2	0.4440	0.4462	0.4430	0.4332	0.4496
1	0.6008	0.6024	0.5933	0.5797	0.6051
0.1	0.9258	0.9238	0.8953	0.8994	0.9147

Table 5.2. Comparison between the variational[9] and numerical[19] results for the drag in plane Couette flow. The last four columns show variational results for different molecular models. The last one, marked with a star, is based on the trial function (5.5.29), the others on (5.5.32).

The relatively poor behavior of the hard sphere model for small Knudsen numbers, where all the models should agree, is due to the fact that, for molecules other than Maxwell's, the term proportional to $\xi_3\xi_1$ does not give an accurate description for small values of Kn and we must modify Eq. (5.5.29) as follows:

$$\tilde{h} = 2\alpha\xi_3 x + \beta L_M^{-1}(\xi_1\xi_3) + \gamma \mathrm{sgn}\,\xi_1)\xi_3 \tag{5.5.32}$$

where α, β and γ are,as before, three adjustable constants to be determined by the variational method and L_M^{-1} the inverse of the usual linearized collision operator. The agreement with the solution obtained by Willis and the variational results for Maxwell molecules, over a wide range of Knudsen numbers, illustrated in Table 5.2, indicates several things, including the accuracy of the BGK model, the usefulness of the variational methods, and the relative insensitivity of the stress in linearized plane Couette flow to the particular molecular model adopted in the calculations.

5.6 Poiseuille Flow

Another interesting flow between parallel plates is plane Poiseuille flow. This is a particular case of various flows in pipes or channels when a pressure difference is present. Since there is no conceptual difference among different shapes, we start by a generic cross section Σ (a strip in the plane case) in the (x, z) plane and assume that there is a small pressure difference in the y direction (Fig. 5.2). We remark that whereas in the continuum regime this pressure drop might arise from a density or a temperature difference, and the results would not differ in the linearized case, the two cases become more and more distinct when the Knudsen number increases. We shall consider the case of a density gradient, since the difference between the two cases is due to a phenomenon called thermal transpiration, which at low Knudsen number is restricted to the Knudsen layers.

Cylindrical Poiseuille flow (Σ is a circle) was carefully investigated by Knudsen in the early part of the 20th century[16]. He found a striking result. If one fixes the pressure difference between the endpoints of a long, narrow tube (a capillary) and lets the average pressure vary, then the flow rate through a cross section of the pipe exhibits a minimum. This phenomenon (known as the Knudsen minimum effect) is somewhat astonishing, because one would expect that the less molecules there are, the smaller will be their flow rate. At the beginning of the 1960s, the matter was still debated and most of the experts thought that there was an error in Knudsen's data and the minimum (a rather flat one) was not there.

Let us see how to attack the problem from a theoretical point of view. We assume the boundaries to be at fixed temperature T_0 and the presence of a small density variation along the y-axis. Then we can look for a solution linearized about a Maxwellian distribution M with a density $\rho = \rho_0 + \rho_1(y)$, with the second and higher order derivatives of smaller order with respect to ρ_1. Then

$$\xi_1 \partial_x h + \xi_2 \partial_y h + \xi_3 \partial_z h + \frac{1}{\rho} \xi_2 \partial_y \rho_1 = L_M h \tag{5.6.1}$$

where we have neglected h when multiplying $\partial_y \rho_1$, as we have done for all the other second order terms. Since we assume that the cross section is independent of y, the dependence of h on y is of second order, because of our assumptions. Thus we can assume h to be constant in y and treat $\partial_y \rho_1/\rho = \partial_y \rho/\rho = k$ as a constant.

Then we have the equation

$$\xi_1 \partial_x h + \xi_3 \partial_z h + k\xi_2 = L_M h. \tag{5.6.2}$$

This equation must be solved with the boundary condition

$$h(x, z, \boldsymbol{\xi}) = 0 \qquad ((x, z) \in \partial\Sigma;\ \xi_1 n_1 + \xi_3 n_3 > 0). \tag{5.6.3}$$

Eq. (5.6.2) holds for the Poiseuille flow in a tube of any cross section Σ. In the plane case the problem reduces to

$$\xi_1 \partial_x h + k\xi_2 = L_M h \tag{5.6.4}$$

with the boundary condition

$$h(x, \boldsymbol{\xi}) = 0 \qquad (x = 0, \xi_1 > 0 \,\text{and}\, x = L, \xi_1 < 0. \tag{5.6.5}$$

The equation to be solved is an inhomogeneous linearized Boltzmann equation, with a source term proportional to ξ_2. If we find a particular solution, then we can subtract it and eliminate the inhomogeneity. To this end, we remark that, since the source does not depend on x, the derivative of any particular solution

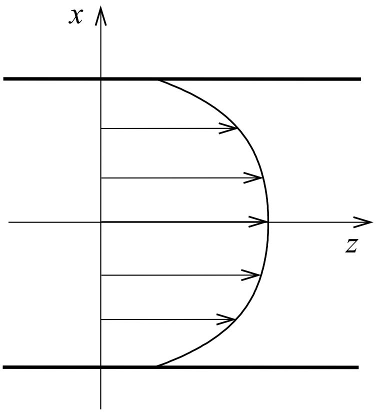

Figure 5.2: Geometry for plane Poiseuille flow. A negative pressure gradient along the y axis causes the gas to move from left to right.

with respect to x will satisfy the homogeneous equation. Since the exponential solutions reproduce themselves by differentiation, the derivative of the simplest particular solution must be a first degree polynomial in x. Hence we look for a particular solution as a second degree polynomial in x. Since the collision invariant multiplying k is x_2, we look for a solution of the form $h_0 = -C\xi_2 x^2 + A(\boldsymbol{\xi})x + B(\boldsymbol{\xi})$ and we expect A and B to be proportional to ξ_2. Here C, and, likewise, D and E (to be soon introduced), are constants. If we insert the last expression into (5.6.4) and equate the coefficients of first and zeroth degree in x in the left- and right-hand side. We obtain

$$-2C\xi_1\xi_2 x = L_M A\,, \qquad A\xi_1 + k\xi_2 = L_M B. \tag{5.6.6}$$

Solving for the first equation, we have $A = -2CL_M^{-1}(\xi_1\xi_2) + D\xi_2$ and the equation for B becomes

$$L_M B = -2C\xi_1 L_M^{-1}(\xi_1\xi_2) + D\xi_2\xi_1 + k\xi_2. \tag{5.6.7}$$

This equation can be solved if and only if the right-hand side is orthogonal to the collision invariants. This condition is trivially satisfied, by symmetry, for all invariants except ξ_2. If we impose that the source in Eq. (5.6.7) is orthogonal to ξ_2 as well, we obtain

$$-2C(\xi_2\xi_1, \xi_2 L_M^{-1}(\xi_1\xi_2)) + k(\xi_2, \xi_2) = 0, \tag{5.6.8}$$

where we have used the notation (g, h) introduced in Section 1. This relation determines C in terms of k. Since $(\xi_2, \xi_2) = RT_0$ and, according to (5.5.13)

$$\mu_0 = -(RT_0)^{-1}(\xi_1 x_2 L_M^{-1}(x_1 x_2))\,, \tag{5.6.9}$$

we have:

$$C = -k(RT_0)^2\mu_0. \tag{5.6.10}$$

Then we obtain from Eq. (5.6.7):

$$B = kL_M^{-1}\left\{\xi_1 L_M^{-1}[(2RT_0)^2\mu_0(\xi_1\xi_2)] + \xi_2\right\} + DL_M^{-1}(\xi_1\xi_2)) + E\xi_2. \tag{5.6.11}$$

Hence we have obtained a particular solution which contains two arbitrary constants, D and E. These will be chosen in such a way as to comply with the symmetry with respect to $x = L/2$ and to simplify the boundary conditions for $h_1 = h - h_0$ as much as possible. This leads to $D = k(RT_0)^2\mu_0$ and $E = 0$. Thus we have

$$\begin{aligned} h_0 = \; & k(RT_0)^2\mu_0\xi_2 x(x-L) + k(RT_0)^2\mu_0 L_M^{-1}(\xi_1\xi_2)(2x-L) \\ & + kL_M^{-1}\left\{\xi_1 L_M^{-1}[(2RT_0)^2\mu_0(\xi_1\xi_2) + \xi_2]\right\}. \end{aligned} \tag{5.6.12}$$

Thus h_1 satisfies the homogeneous linearized Boltzmann equation and the boundary conditions

$$h_1(x,\boldsymbol{\xi}) = -2k(RT_0)^2\mu_0 L_M^{-1}(|\xi_1|\xi_2) + kL_M^{-1}\left\{\xi_1 L_M^{-1}[(2RT_0)^2\mu_0(\xi_1\xi_2)] + \xi_2\right\}$$

$$(x = 0,\ \xi_1 > 0 \text{ and } x = L,\ \xi_1 < 0). \tag{5.6.13}$$

We remark that for large values of the Knudsen number, the part of the solution arising from h_0 will dominate and we shall obtain the familiar parabolic profile. The flow rate will be, for fixed values of L and the pressure difference, inversely proportional to the Knudsen number Kn and hence will increase for an increasing average pressure.

However, this behavior will not be always correct, because of the increasing role played by the Knudsen layers. In order to see what happens at low pressures, we remark that for free-molecular conditions, Eq. (5.6.4) formally reduces to

$$\xi_1\partial_x h + k\xi_2 = 0 \tag{5.6.14}$$

or, if we take into account the boundary conditions,

$$h = -k\xi_2\left(\frac{x - L/2}{\xi_1} + \frac{L/2}{|\xi_1|}\right). \tag{5.6.15}$$

A singularity at $\xi_1 = 0$ is apparent. We know, however, that molecules travelling almost parallel to the walls or with extremely low speeds are not well described by this equation, because they, no matter how few molecules there are around, will collide more frequently with other molecules than with the wall. Thus Eq. (5.6.2) can be assumed to hold for $|\xi_1| \geq (RT_0)^{1/2}/\text{Kn}$. Otherwise we have to compute the effect of the molecular collisions, which will change abnormally low values of ξ_1. Then we can compute the bulk velocity by integrating over the molecules having a value of ξ_1 satisfying the above restriction, since for the others the solution is not good. We find:

$$\begin{aligned} \rho v &= \int_{\xi_1 \leq (RT_0)^{1/2}/\mathrm{Kn}} Mh d\boldsymbol{\xi} = -\frac{\partial \rho}{\partial y} \frac{LRT_0}{2} \int_{|\xi_1| \geq (RT_0)^{1/2}/\mathrm{Kn}} \frac{\exp(-\xi_1^2/2RT_0)}{|\xi_1|} d\xi_1 \\ &= -\frac{\partial \rho}{\partial y} LRT_0 \log(\mathrm{Kn}) + O(1) \end{aligned} \tag{5.6.16}$$

where $O(1)$ denotes a term which remains finite when the Knudsen number goes to ∞.

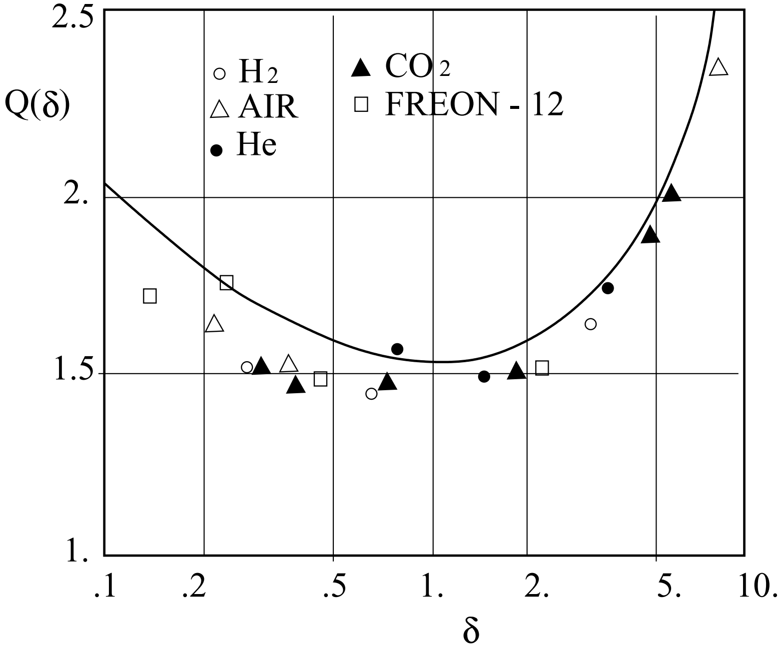

Figure 5.3: Normalized flow rate in plane Poiseuille flow. Comparison between the variational solution and Dong's data. The presence of a minimum is clear.

The first order effects of collisions will be to remove the molecules which would make v infinity and the above estimate is correct. A detailed study has been carried out for the BGK model by using either the method of collision iteration[10] or a method based on the exact solution[11], and confirms the estimate in Eq. (5.6.16). Thus the flow rate diverges for Kn$\to \infty$. This behavior confirms that the flow rate must have at least one minimum, since it decreases for small average pressure and increases for large average pressures.

Actually for a slab, the minimum is rather more marked than in a cylindrical pipe and even rough calculations[10] indicate that it must occur for Kn$\cong$ 1. More accurate results can be obtained with the finite ordinate schemes of the kind mentioned in Section 4. The second scheme can be shown to approximate the solution from above while the first appears to approximate the solution from below. The minimum appears to be located at approximately Kn= 1.1. Calculations with the variational method have also been made[13], since the flow rate is naturally related to the functional to be minimized.

It is not possible, of course, to make experiments in a real slab, but experimental data for a channel with a rather thin rectangular cross section are available[22]. Provided we keep the Knudsen number not too large, in order to avoid the effects of the finite width of the channel, it is possible to make a comparison, which shows a good agreement between theory and experiment (see Fig. 5.3).

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Chapter 6

Flows in More Than One Dimension

6.1 Introduction

In the previous chapter we have learned the basic tools required to deal with problems in rarefied gas dynamics. Some of them can be readily extended to problems in more than one dimension (actually, occasionally we presented these tools in a general form, when this did not reduce the clarity of exposition).

In this chapter we first study the extension of the techniques to handle the linearized Boltzmann equation to the case of geometries different from a slab or a half-space. The results on the general solution in the one-dimensional case, suitably modified will give a general idea of the solution in three dimensions (Section 2). Then we shall discuss particular cases of both internal (Section 3) and external (Section 4) steady flow problems.

This will naturally lead to a general discussion of the continuum limit of the Boltzmann equation.

6.2 Linearized Steady Problems

In this section we shall examine the linearized Boltzmann equation and study the general form of its solution in 3-dimensional steady problems.

We start from the remark that sometimes it is convenient to consider two solutions of the linearized Boltzmann equation simultaneously. We consider these solutions in the steady case and denote them by h and $h^{\dagger}$. In order to reach more generality we consider the presence of a source (as in the case of Poiseuille flow, see Section 3.4) for each solution and we denote them by S and $S^{\dagger}$. Then we write

$$Dh = Lh + S, \tag{6.2.1}$$

$$Dh^\dagger = Lh^\dagger + S^\dagger \,, \tag{6.2.2}$$

where $D = \boldsymbol{\xi} \cdot \partial_{\mathbf{x}}$ and L the linearized collision operator about some fixed, non-drifting Maxwellian distribution M. We also use the parity operator P and adopt the notations $((\cdot,\cdot))$ and $((\cdot,\cdot))_B$ introduced in Section 5.5. Then we have:

$$\begin{aligned}((Ph^\dagger, S)) - ((h, PS^\dagger)) &= ((Ph^\dagger, (D-L)h)) - ((h, P(D-L)h^\dagger)) \\ &= ((Ph^\dagger, Dh)) - ((h, PDh^\dagger))\,,\end{aligned} \tag{6.2.3}$$

where we used the property

$$((Pg, Lh)) = ((LPg, h)) = ((PLg, h)) = ((h, PLg))$$

that we discussed in Chapter 5 to eliminate the terms containing the linearized collision operator L. The terms which have been left over can be clearly transformed into boundary terms, as we did in Chapter 5. Then we obtain

$$((Ph^\dagger, S)) - ((h, PS^\dagger)) = ((h^{\dagger +}, Ph^-))_B - ((h^+, Ph^{\dagger -}))_B\,. \tag{6.2.4}$$

This is a general relation between the solutions h, $h^\dagger$ and their sources S, $S^\dagger$.

A particular case of interest is offered by the choice

$$S^\dagger = \delta(\mathbf{x} - \mathbf{x}')\delta(\boldsymbol{\xi} - \boldsymbol{\xi}')\,, \tag{6.2.5}$$

where, as usual, δ denotes Dirac's delta function. The corresponding solution is denoted by $G(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}'), \boldsymbol{\xi}')$ and is called the Green's function (in the absence of boundaries, if we choose that Eq. (6.2.2) is satisfied in the entire space with suitable conditions at infinity). If h is a solution satisfying Eq. (6.2.1) in some region Ω with boundary conditions of the usual kind on the boundary $\partial\Omega$, Eq. (6.2.4) becomes

$$\begin{aligned}&\int_{\Re^3}\int_\Omega G(\mathbf{x}, -\boldsymbol{\xi}; \mathbf{x}', \boldsymbol{\xi}')S(\mathbf{x}, \boldsymbol{\xi})M(|\boldsymbol{\xi}|)d\mathbf{x}d\boldsymbol{\xi} - h(\mathbf{x}', -\boldsymbol{\xi}')M(|\boldsymbol{\xi}'|) \\ &= -\int_{\Re^3}\int_{\partial\Omega} \boldsymbol{\xi}\cdot\mathbf{n}G(\mathbf{x}, -\boldsymbol{\xi}; \mathbf{x}', \boldsymbol{\xi}')h(\mathbf{x}, \boldsymbol{\xi})M(|\boldsymbol{\xi}|)d\sigma d\boldsymbol{\xi}\,,\end{aligned} \tag{6.2.6}$$

or, rearranging,

$$\begin{aligned}h(\mathbf{x}, \boldsymbol{\xi})M(|\boldsymbol{\xi}|) = &\int_{\Re^3}\int_\Omega G(\mathbf{x}', -\boldsymbol{\xi}'; \mathbf{x}, -\boldsymbol{\xi})S(\mathbf{x}', \boldsymbol{\xi}')M(|\boldsymbol{\xi}'|)d\mathbf{x}d\boldsymbol{\xi} \\ &+ \int_{\Re^3}\int_{\partial\Omega} \boldsymbol{\xi}'\cdot\mathbf{n}'G(\mathbf{x}', -\boldsymbol{\xi}'; \mathbf{x}, -\boldsymbol{\xi})h(\mathbf{x}', \boldsymbol{\xi}')M(|\boldsymbol{\xi}'|)d\sigma d\boldsymbol{\xi}'\,.\end{aligned} \tag{6.2.7}$$

This equation shows that the solution h of Eq. (6.2.1) can be expressed in terms of the source S and the boundary values of h on $\partial\Omega$, once G is known. The problem is, of course, that the boundary values are not known (in the simplest case, they are known for $\boldsymbol{\xi}'\cdot\mathbf{n} > 0$, but not for $\boldsymbol{\xi}'\cdot\mathbf{n} < 0$). It is possible, using the Green's function, to obtain integral equations that determine the boundary values. Because of the translation invariance of Eq. (6.2.1), G will actually depend just on the combination $\mathbf{x}-\mathbf{x}'$ and not separately on $\mathbf{x}$ and $\mathbf{x}'$. Taking this remark into account and exchanging $\mathbf{x}$ and $\mathbf{x}'$, $\boldsymbol{\xi}$ and $\boldsymbol{\xi}'$ simultaneously:

$$G(\mathbf{x}, -\boldsymbol{\xi}; \mathbf{x}', -\boldsymbol{\xi}') = G(\mathbf{x}', \boldsymbol{\xi}'; \mathbf{x}, \boldsymbol{\xi})\,. \tag{6.2.8}$$

Then Eq. (6.2.7) can be slightly simplified to

$$\begin{aligned} h(\mathbf{x}, \boldsymbol{\xi})M(|\boldsymbol{\xi}|) = &\int_{\Re^3}\int_{\Omega} G(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}', \boldsymbol{\xi}')S(\mathbf{x}', \boldsymbol{\xi}')M(|\boldsymbol{\xi}'|)d\mathbf{x}d\boldsymbol{\xi}' \\ &+ \int_{\Re^3}\int_{\partial\Omega} \boldsymbol{\xi}' \cdot \mathbf{n}' G(\mathbf{x}, \boldsymbol{\xi}; \mathbf{x}', \boldsymbol{\xi}')h(\mathbf{x}', \boldsymbol{\xi}')M(|\boldsymbol{\xi}'|)d\sigma' d\boldsymbol{\xi}'\,. \end{aligned} \tag{6.2.9}$$

In spite of the fact that Eq. (6.2.9) still contains unknown boundary values, it can give us information on the structure of the solutions of the linearized Boltzmann equation, provided we know G. In particular, if the source S is absent, the solution inside Ω will depend on $\mathbf{x}$ in the same way as G does, because only the boundary integral will survive and $\mathbf{x} \neq \mathbf{x}'$ in Ω.

Let us then look at the structure of the Green's function. Since we know that G depends on just the combination $\mathbf{x} - \mathbf{x}'$, we can let $\mathbf{x}' = 0$ without loss of generality and write $G(\mathbf{x}, \boldsymbol{\xi}; \boldsymbol{\xi}')$ for $G(\mathbf{x}, \boldsymbol{\xi}; 0, \boldsymbol{\xi}')$. We have then to solve the equation

$$\boldsymbol{\xi} \cdot \partial_{\mathbf{x}} G = LG + \delta(\mathbf{x})\delta(\boldsymbol{\xi} - \boldsymbol{\xi}')\,. \tag{6.2.10}$$

A suitable method is to take the Fourier transform with respect to $\mathbf{x}$:

$$\hat{G}(\mathbf{k}, \boldsymbol{\xi}; \boldsymbol{\xi}') = \int G(\mathbf{x}, \boldsymbol{\xi}; \boldsymbol{\xi}')e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}\,, \tag{6.2.11}$$

inverted by

$$G(\mathbf{x}, \boldsymbol{\xi}; \boldsymbol{\xi}') = \frac{1}{2\pi}\int \hat{G}(\mathbf{k}, \boldsymbol{\xi}; \boldsymbol{\xi}')e^{-i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k}\,. \tag{6.2.12}$$

Then Eq. (6.2.10) gives

$$-i\boldsymbol{\xi} \cdot \mathbf{k}\hat{G} = L\hat{G} + \delta(\boldsymbol{\xi} - \boldsymbol{\xi}')\,. \tag{6.2.13}$$

Here $\mathbf{k}$ is just a (vector-valued) parameter. If we let $\xi_1 = \boldsymbol{\xi}\cdot\mathbf{k}/|\mathbf{k}|$ ($\mathbf{k} \neq 0$), we have

$$-i\xi_1|\mathbf{k}|\hat{G} = L\hat{G} + \delta(\boldsymbol{\xi} - \boldsymbol{\xi}')\,. \tag{6.2.14}$$

Then we are reduced to finding the Green's function in the one-dimensional case, where the other two components of $\boldsymbol{\xi}$ form a vector in the plane orthogonal to $\mathbf{k}$. From the general solution for one-dimensional problems, a lengthy but simple calculation leads to the Green's function for this case, G_1. We have:

$$G_1 = \left\{ \frac{\xi_1' + \xi_1}{2C_1} + \sum_{\alpha=2}^{4} \frac{\psi_\alpha [L^{-1}(\xi_1\psi_\alpha)]' + \psi_\alpha' [L^{-1}(\xi_1\psi_\alpha)]}{2C_\alpha} \right\} \operatorname{sgn} x + \sum_{\alpha=2}^{4} \frac{\psi_\alpha \psi_\alpha' |x|}{2C_\alpha}$$
$$+ \operatorname{sgn} x \int_{\overline{\gamma}}^{\infty} g_\gamma(\boldsymbol{\xi}) g_\gamma(\boldsymbol{\xi}') \exp(-\gamma|x|) d\gamma \,. \tag{6.2.15}$$

In order to pass to the 3D-case one must be careful, because of the contribution from $\mathbf{k} = 0$. Thus it is better to split the contribution from the discrete terms and from the integral. The latter poses no problems and provides a solution that decays exponentially when going far from the source. The Fourier transforms of the discrete terms are singular; in addition, the transformation from the 3D- to the 1D-case is singular for $|\mathbf{k}| = 0$. In order to avoid difficulties and possible mistakes we deal with the contribution not decaying exponentially directly, using the remark that it can be expanded, at least asymptotically, in powers of the mean free path. Thus we have

$$h = h^A + h^B \,, \tag{6.2.16}$$

where h^B is important near boundaries and h^A survives also far from the boundaries (the asymptotic part) and hence cannot depend exponentially on $\mathbf{x}/\ell$ where ℓ is the mean free path.

In order to compute h^A we proceed as follows. We write

$$h^A = \sum_{\alpha=1}^{4} A_\alpha(\mathbf{x})\psi_\alpha + \epsilon A_0(\mathbf{x}) + \epsilon L^{-1} \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} h^A \,, \tag{6.2.17}$$

where, as before (Chapter 5), $\psi_4 = |\boldsymbol{\xi}|^2 - 5RT_0$ and we have taken into account the fact that the term with $\psi_0 = 1$ must be of order ϵ when we iterate because $\psi_0 \boldsymbol{\xi}$ is not orthogonal to the collision invariants. If we now iterate, we obtain

$$h^A = \sum_{\alpha=1}^{4} A_\alpha(\mathbf{x})\psi_\alpha + \epsilon A_0(\mathbf{x}) + \epsilon L^{-1} \sum_{\alpha=1}^{4} \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} A_\alpha(\mathbf{x})\psi_\alpha + \epsilon^2 L^{-1} [\boldsymbol{\xi} \cdot \partial_{\mathbf{x}} A_0$$
$$+ \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} L^{-1} \cdot \boldsymbol{\xi} \partial_{\mathbf{x}} h^A] \,. \tag{6.2.18}$$

We must now impose the condition that $\boldsymbol{\xi} \cdot \partial_{\mathbf{x}} A_0 + \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} L^{-1} \sum_{\alpha=1}^{4} \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} A_\alpha(\mathbf{x})\psi_\alpha$ is orthogonal to the collision invariants (otherwise we cannot continue the iteration).

If we repeat the procedure we get more and more terms. We are not interested in obtaining all the terms of the expansion (which presumably is not convergent, in general, but only asymptotic). The important fact is that, if we compute moments of fixed order (such as the stress tensor and the heat flow), a finite number of terms will be needed. To see this we remark that h will depend linearly on $\mathbf{x}$ only through the five quantities $A_\alpha(\mathbf{x})$, or p_1^A, $\mathbf{v}_1^A$, T_1^A (the perturbations of pressure, bulk velocity and temperature). Then a tensor of a given order can depend on just certain combinations of the derivatives of these quantities (because the rotational invariance of the collision term implies that a monatomic Boltzmann gas is an isotropic medium). The heat flow $\mathbf{q}$ is a linear combination with constant coefficients of

$$\partial_{\mathbf{x}} p_1^A,\ \partial_{\mathbf{x}} T_1^A,\ \partial_{\mathbf{x}} \Delta^n p_1^A,\ \partial_{\mathbf{x}} \Delta^n T_1^A,\ \Delta^n \mathbf{v}_1^A \qquad \text{(q)}\,,$$

where Δ is the Laplace operator and $n = 1, 2, 3, \ldots$. The stress deviator $q_{ij} = p_{ij} - p\delta_{ij}$ is a linear combination with constant coefficients of

$$\partial_{x_j} u_{1i}^A,\ \partial_{x_j} \Delta^n u_{1i}^A,\ \partial_{x_i x_j} p_1^A,\ \partial_{x_i x_j} T_1^A,\ \partial_{x_i x_j} \Delta^n p_1^A,\ \partial_{x_i x_j} \Delta^n T_1^A \qquad \text{(p)}\,.$$

The coefficients of a term containing derivatives of order m are of order ϵ^m at least. Now we recall the balance equation which must be satisfied as a consequence of the existence of the collision invariants:

$$\begin{gathered} \operatorname{div} \mathbf{v}_1^A = 0, \\ \partial_{x_i} p^A = \sum_{i=1}^{3} \partial_{x_j} q_{ij} \quad (i = 1, 2, 3), \\ \operatorname{div} \mathbf{q} = 0\,. \end{gathered} \tag{6.2.19}$$

If we take into account the last relation we see that the left hand side will contain a linear combination of terms of the following kind:

$$\Delta p_1^A,\ \Delta T_1^A,\ \Delta^{n+1} p_1^A,\ \Delta^{n+1} T_1^A\,,$$

because the terms containing $\mathbf{v}_1^A$ will disappear since their divergence is zero.

The momentum balance equation will contain in the right-hand side terms of the following kind:

$$\Delta u_{1i}^A,\ \Delta^{n+1} u_{1i}^A,\ \partial_{x_i} \Delta p_1^A,\ \partial_{x_i} \Delta T_1^A,\ \partial_{x_i} \Delta^{n+1} p_1^A,\ \partial_{x_i} \Delta^{n+1} T_1^A\,.$$

The momentum equation shows that the pressure gradient can be omitted from the variables upon which $\mathbf{q}$ depends, because it can be expressed in terms of other variables appearing in the list (q). Thus ΔT_1^A is a linear combination of $\Delta^{n+1} p_1^A,\ \Delta^{n+1} T_1^A$. Taking the divergence of the momentum equation, we see that also Δp_1^A is a linear combination of $\Delta^{n+1} p_1^A,\ \Delta^{n+1} T_1^A$. Then ΔT_1^A and Δp_1^A must vanish, otherwise they would have an exponential change on the scale of a mean free path, which we have excluded. Thus

$$\Delta p_1^A = 0, \quad \Delta T_1^A = 0\,, \tag{6.2.20}$$

and the right-hand side of the momentum equation will just contain

$$\Delta u_{1i}^A,\ \Delta^{n+1} u_{1i}^A\,.$$

Taking the Laplacian of the same equation we obtain, since $\Delta p_1^A = 0$, that a linear combination of terms of the form $\Delta^{n+1} u_{1i}^A$ ($n = 1, 2, 3, \ldots$) vanishes. Again, $\Delta^2 u_{1i}^A = 0$, because $\Delta^2 u_{1j}^A$ cannot have an exponential change on the scale of the mean free path. Then the momentum equation reduces to

$$\partial_{x_i} p = \mu \Delta u_{1i}^A \quad (i = 1, 2, 3)\,. \tag{6.2.21}$$

We conclude that the stress deviator and the heat flow have the following form:

$$q_{ij} = -\mu(\partial_{x_j} u_{1i}^A + \partial_{x_i} u_{1j}^A) + \sigma \partial_{x_i x_j} T_1^A\,, \tag{6.2.22}$$

$$\mathbf{q} = -\kappa \partial_{\mathbf{x}} T_1^A + \tau \Delta \mathbf{v}_1^A\,, \tag{6.2.23}$$

where $\mu, \sigma, \kappa, \tau$ are four coefficients of the order of the mean free path. In particular, the momentum balance equations take on the form given above, Eq. (6.2.21). The most important change with respect to traditional continuum mechanics is the presence of the term with the second derivatives of temperature in the expression of the stress deviator and of the term with the second derivatives of bulk velocity in the expression of the heat flow. These terms were already known to Maxwell[13]. In recent times, their importance has been stressed by Kogan *et al.*[12] and by Sone *et al.*[16,17]. Approximate values of σ and τ are given in Ref. 17.

Summarizing, the solution of the linearized Boltzmann equation reduces to the sum of two terms, one of which, h^B, is important just in the Knudsen layers and the other, h^A, is important far from the boundaries. The latter has a stress deviator and a heat flow given by Eqs. (6.2.22–23). We remark that, although these constitutive equations are different from those of Navier–Stokes and Fourier, the bulk velocity, pressure, and temperature satisfy the Navier–Stokes equations. In fact, when we take the divergence of the heat flow vector the term proportional to the Laplacian of $\mathbf{v}$ vanishes, thanks to the continuity equation, and thus just the term proportional to the temperature gradient survives; then, taking the divergence of the stress, the term $\mathrm{grad}(\Delta T_1^A)$ vanishes, because of the energy equation. Yet, the new terms in the constitutive relations may produce physical effects in the presence of boundary conditions different from those of no-slip and no temperature jump. In fact we must expect the velocity slip to be proportional to the shear stress and the temperature jump to the heat flow.

There are however flows where the agreement between the Boltzmann equation and the Navier–Stokes equations does not occur even at small Knudsen numbers. These flows will be discussed in Section 5.

6.3 Linearized Solutions of Internal Problems

The typical internal problems in more than one dimension are the flow in pipes (possibly with annular cross-section), or between two coaxial rotating cylinders or spheres.

The simplest case is offered by Poiseuille flow in a pipe of arbitrary cross section. The starting point is Eq. (5.6.2). If we adopt the BGK model, we can obtain an integral equation for the bulk velocity $v_2(\mathbf{x})$, where $\mathbf{x}$ is the two-dimensional vector describing the cross-section of the pipe divided by the mean free path $\ell = 2\pi^{-1/2}\lambda$. If we let $v_2(\mathbf{x}) = (RT_0/2)^{1/2}\ell p^{-1}(dp/dy)(1-\phi(\mathbf{x}))$, the integral equation to be solved can be written as

$$\phi(\mathbf{x}) = 1 + \pi^{-1}\int_{\Sigma(\mathbf{x})} T_0(|\mathbf{x}-\mathbf{y}|)|\mathbf{x}-\mathbf{y}|^{-1}\phi(\mathbf{y})\mathrm{d}\mathbf{y}\,. \tag{6.3.1}$$

This equation can be solved numerically for any given cross section; two cases which have been actually considered are the case of a circular cross section[4] and the case of an annulus[1]. Another method is the variational one. The functional to be considered is

$$J(\tilde{\phi}) = \int_{\Sigma}[\tilde{\phi}(\mathbf{x})]^2\mathrm{d}\mathbf{y} - \pi^{-1}\int_{\Sigma}\int_{\Sigma(\mathbf{x})} T_0(|\mathbf{x}-\mathbf{y}|)|\mathbf{x}-\mathbf{y}|^{-1}\tilde{\phi}(\mathbf{y})\tilde{\phi}(\mathbf{x})\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{x} - 2\int_{\Sigma}\tilde{\phi}(\mathbf{x})\mathrm{d}\mathbf{x}\,. \tag{6.3.2}$$

This functional attains its minimum value when $\tilde{\phi} = \phi$ (the solution of Eq. (6.3.1)). This value is

$$J(\phi) = -\int_{\Sigma}\phi(\mathbf{x})\mathrm{d}\mathbf{x}\,, \tag{6.3.3}$$

a quantity obviously related to the flow rate.

δ	$Q(\delta)^4$	$Q(\delta)^5$
10	3.5821	3.5573
7	2.8440	2.8245
5	2.3578	2.3438
4	2.1188	2.1079
3	1.8850	1.8772
2	1.6608	1.6559
1.6	1.5753	1.5722
1.4	1.5348	1.5321
1.2	1.4959	1.4937
1.0	1.4594	1.4576
0.8	1.4261	1.4247
0.6	1.3982	1.3971
0.4	1.3796	1.3788
0.2	1.3820	1.3815
0.1	1.4043	1.4039
0.01	1.4768	1.4801

Table 6.1. Comparison between the variational[5] and numerical[4] results for the nondimensional flow rate in cylindrical Poiseuille flow.

As in the case of a slab, one can obtain very accurate results by inserting the parabolic profile (which becomes exact in the continuum limit). At variance with the plane case, we have to evaluate double integrals; only one of the quadratures can be performed in closed form, whereas one has to resort to numerical methods to complete the calculations[5]. Table 6.1 gives a comparison for the results for the flow rate as supplied by the two methods (numerical solution[4] and variational method[5]). The agreement is very good. The theoretical results also compare very well with the experimental data (Fig. 6.1). In particular, the flow rate exhibits a minimum for a value of the ratio δ between the radius of the cylinder and the mean free path ℓ close to 0.3, in excellent agreement with experimental data. The values of the flow rate show a maximum deviation of the order of 3% from experimental data.

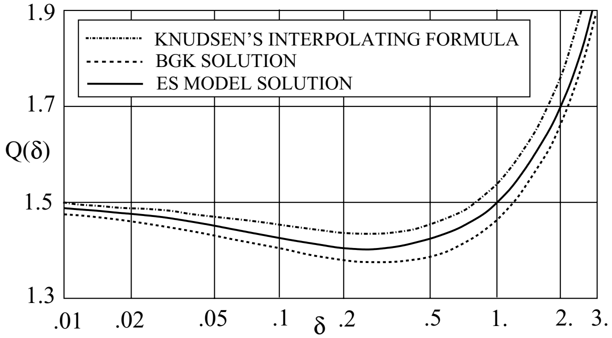

Figure 6.1: Comparison between theory and experiment for cylindrical Poiseuille flow. Here δ is the ratio of the radius a of the cylinder to the mean free path λ and Q the ratio between the mass flow rate and $-\pi a^2(2RT)^{-1/2}(dp/dz)$.

We remark that the problem of cylindrical Poiseuille flow can be treated by using the ES model[6] to show that the corresponding solution can be obtained from the solution for the BGK model by a simple transformation. For the flow rate the formula takes the form[7]

$$Q(\delta, \mathrm{Pr}) = Q(\delta\,\mathrm{Pr}, 1) + (1 - \mathrm{Pr})\frac{\delta}{4} \tag{6.3.4}$$

where $Q(\delta\,\mathrm{Pr}, 1)$ is, of course, given by the solution of the BGK model. If the value $\mathrm{Pr} = 2/3$ is chosen, as is appropriate for a monatomic gas, the disagreement between the experimental data and the theoretical curve reduces to 1 or 2%. This is shown in Fig. 6.1, taken from Ref. 6.

Other important problems which can be solved with little effort by using the linearized BGK model equation are the Couette flow between two concentric cylinders[8] and the heat transfer between two concentric cylinders[2].

In all the solutions of the problems discussed above, the boundary conditions are those of diffuse reflection according to a Maxwellian distribution.

6.4 External Problems

If we use the linearized Boltzmann equation the problem of finding the flow past a body does not have a solution in two dimensions, because it is impossible to match a nonzero flow at infinity since the solutions diverge logarithmically[9]. We shall examine this matter in the next section. On the other hand, the solution of three-dimensional problems is amenable to a numerical or variational treatment. A rigorous proof that the linearized solutions supply a good approximation for the nonlinear problem of the flow past a body at low speeds is supplied by the proofs of convergence of the perturbation series by Ukai and Asano[19].

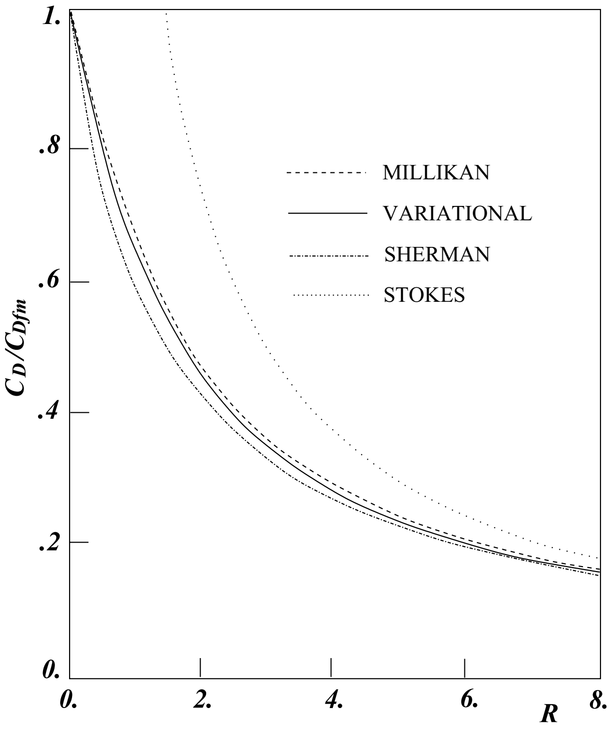

Figure 6.2: Low speed drag coefficient of a sphere versus the nondimensional radius R. Millikan's curve interpolate his experimental data

The most interesting problem is the flow past a sphere. This is a classical problem since Millikan derived experimental data for the drag on a sphere at low speeds, with the purpose of using them in his celebrated oil drop experiments to measure the electron charge[14]. In this experiment a spherical drop of very small size (aerosol) is under the action of an electric field, of gravity and of the drag exerted by air.

A variational calculation of the drag was performed by Cercignani, Pagani and Bassanini[10] with the BGK model. The agreement with experimental data is excellent. This is shown in Fig. 6.2, where the results obtained with the Stokes equations (this is the name usually given to the linearized Navier–Stokes equation) and the interpolating formula by Sherman[15] are also shown. The latter is a universal formula which relates a generic quantity $F(\mathrm{Kn})$, a function of the Knudsen number Kn, to its free-molecular limit F_{FM} and its value according to continuum mechanics $F_C(\mathrm{Kn})$, provided $F_C(\mathrm{Kn})/F_{FM} \to 0$ as $\mathrm{Kn} \to 0$. Sherman's general formula reads as follows[15]:

$$\frac{F(\mathrm{Kn})}{F_{FM}} = \left(1 + \frac{F_{FM}}{F_C(\mathrm{Kn})}\right)^{-1}, \tag{6.4.1}$$

and in the case of the drag on a sphere becomes

$$C_D(R) = [1 + (0.685)R]^{-1}, \tag{6.4.2}$$

where R is a suitable inverse Knudsen number, the ratio between the radius of the sphere and the mean free path ℓ.

As Fig. 6.2 shows, the Navier–Stokes equations are completely wrong for values of R of about 10 or less. The variational BGK results[10] are in excellent agreement with the formula provided by Millikan to interpolate his experimental data[14]. Sherman's formula is in a reasonably good agreement with the data. The same agreement of this simple interpolation occurs for other typical quantities, with the remarkable exception of the flow rate for Poiseuille flow (no minimum is exhibited by Sherman's formula[15]).

Another problem which can be treated with the variational method is the heat transfer from a sphere[5]. Here, following Sherman, the ratio of the heat flow q to its free-molecular limit is plotted against the ratio of the value of the same heat flow according to continuum mechanics q_c and q_0. The agreement with the data by Takao[18] at $\mathrm{M} = 0$ and by Kavanau[11] at various values of the Mach number ranging from $\mathrm{M} = 0.1$ to $\mathrm{M} = 0.69$ is remarkable.

An exception to the aforementioned difficulty with 2-dimensional problems is offered by the flow produced by a rotating cylinder in an infinite expanse of gas, which is at rest at space infinity. In this case the BGK solution can be easily obtained numerically[3]; an approximate analytical solution has also been produced[3]. This solution is in a better agreement with the numerical solution than a four-moment solution by Willis[21].

In all the problems discussed above, the boundary conditions are those of diffuse reflection according to a Maxwellian distribution.

6.5 The Stokes Paradox in Kinetic Theory

Here we shall discuss the difficulty mentioned at the beginning of the previous section for external flows in two dimensions. Let us consider a steady flow problem past a solid body. The body is finite, at rest and kept at uniform temperature. The boundary conditions are of the general kind, linear and homogeneous, discussed in Section 4.1. Thus, unless the boundary conditions are deterministic, there is a Maxwellian distribution M_0, uniquely determined up to a factor, which satisfies the boundary conditions. At space infinity the distribution function is assumed to tend to another Maxwellian distribution M_∞. We linearize the Boltzmann equation with respect to M_0, made unique by choosing its density to be the same as that of M_∞. In the case of specular and reverse reflection we need to fix more things to make the Maxwellian distribution unique; we choose the temperature to be the same as that in M_∞ and a vanishing drift velocity. Then we try to find a solution linearized with respect to M_0.

The linearized Boltzmann equation may be written as follows:

$$\boldsymbol{\xi} \cdot \partial_{\mathbf{x}} h = Lh(\mathbf{x}, \boldsymbol{\xi}) \,, \tag{6.5.1}$$

where $\mathbf{x}$ varies in some region Ω outside a finite, smooth region of ordinary space and $\boldsymbol{\xi}$ in the entire velocity space.

We shall assume that h tends to a collision invariant *uniformly* when $|\mathbf{x}| \to \infty$, as seems reasonable (far from the boundary the solution of the linearized Boltzmann equation is very smooth, except, possibly, in a zero measure set where the solution is discontinuous, the discontinuity going to zero when $R \to \infty$).

Following Ref. 9, we want to show that *if*

$$\int_{\partial\Omega_2} \boldsymbol{\xi} \cdot \mathbf{n} h^2 d\boldsymbol{\xi} d\sigma \to 0 \tag{6.5.2}$$

when the closed surface $\partial\Omega_2$ tends to infinity, then h must be a constant.

The linearized version of the Boltzmann inequality reads as follows (Section 1.10):

$$\int_{\Re^3} hLhd\boldsymbol{\xi} \leq 0 \,, \tag{6.5.3}$$

the equality sign holding if, and only if, h is a collision invariant.

Let us consider now a bounded region Ω_{12} between two finite surfaces, one inside the other and both outside Ω. The external surface will be called $\partial\Omega_2$ and the internal one $\partial\Omega_1$.

Let us multiply Eq. (6.5.1) and integrate with respect to both $\boldsymbol{\xi}$ and $\mathbf{x}$, the latter integration being restricted to Ω_{12}. Then, because of Eq. (6.5.3), we have

$$\int_{\partial\Omega_{12}} \boldsymbol{\xi} \cdot \mathbf{n} h^2 d\boldsymbol{\xi} d\sigma \leq 0 \,, \tag{6.5.4}$$

where $\mathbf{n}$ is the outward normal. Here equality holds if, and only if, h is a collision invariant.

We now decompose $\partial\Omega_{12}$ into the two disconnected parts $\partial\Omega_1$ and $\partial\Omega_2$ and orient both normal unit vectors toward space infinity. Then Eq. (6.5.4) may be rewritten as

$$\int_{\partial\Omega_2} \boldsymbol{\xi}\cdot\mathbf{n}h^2 d\boldsymbol{\xi} d\sigma \le \int_{\partial\Omega_1} \boldsymbol{\xi}\cdot\mathbf{n}h^2 d\boldsymbol{\xi} d\sigma\,. \tag{6.5.5}$$

If we let the outer surface go to infinity, the corresponding integral will tend to zero, because of our assumption; then we can say, since Eq. (6.5.5) holds whenever $\partial\Omega_2$ encloses $\partial\Omega_1$, that both integrals are nonnegative. Letting $\partial\Omega_1$ tend to $\partial\Omega$, Eq. (6.5.5) then becomes

$$0 \le \int_{\partial\Omega_2} \boldsymbol{\xi}\cdot\mathbf{n}h^2 d\boldsymbol{\xi} d\sigma \le \int_{\partial\Omega} \boldsymbol{\xi}\cdot\mathbf{n}h^2 d\boldsymbol{\xi} d\sigma\,, \tag{6.5.6}$$

where now $\partial\Omega_2$ is any closed surface enclosing $\partial\Omega$. Because of the properties of the kernel appearing in the boundary conditions (see Section 4.1), the last integral is nonpositive and we obtain that both integrals in Eq. (6.5.6) must vanish. Because of the arbitrariness of $\partial\Omega_2$, this implies that the vector $\int_{\Re^3} \boldsymbol{\xi} h^2 d\boldsymbol{\xi}$ is divergence-free outside Ω. Then, because of Eqs. (6.5.1) and (6.5.3), we obtain

$$\int_{\Re^3} hLh d\boldsymbol{\xi} = 0\,, \tag{6.5.7}$$

which implies that h is a collision invariant.

We must now impose the condition that this collision invariant is a steady solution of the linearized Boltzmann equation and satisfies the boundary conditions. It is easy to show that this is possible if and only if h is a constant.

This result has been obtained under certain assumptions. One of them, expressed by Eq. (6.5.2) is not obvious. The physical meaning of this assumption is that there is no entropy source (or sink) at space infinity , but the result would hold even if we allow entropy production at space infinity. Thus there must be an entropy sink there, which swallows the entropy produced near the body.

In order to investigate whether this is compatible with the behavior of the solutions of the linearized Boltzmann equation, we remark that far from the body the Stokes equations must hold, because of the discussion in Section 2. Then the situation in three dimensions is satisfactory, since the Stokes solution is known to be well-behaved at infinity[20], in the sense that it approaches a uniform flow.

The situation is not equally satisfactory in the plane case; in fact, to exemplify, in the case of an axisymmetric body, assuming the temperature to be the same at space infinity and on the surface of the body, the expressions for the pressure and the bulk velocity contain terms of degrees 0, -1 and terms of lower degrees in the distance r from a point inside the body[20]. The last ones cannot change the limiting behavior of the entropy flow. The constant in the pressure, under our assumptions, is zero. The viscous stresses, evaluated with the Navier–Stokes formula, obviously turn out to be of the same order as the pressure. The temperature is completely uncoupled from the other quantities. In any case, if the temperature is bounded, the heat flow must decrease more rapidly than r^{-1}, according to Fourier's law. Thus the leading contribution to the integral in the left-hand side of Eq. (6.5.2) is proportional to a linear combination of the surface integrals of $\sum_{i,j=1}^{3} p_{jk}u_j n_k$ and q_n/T_0, which are both of order smaller than r^{-1}. and hence produce a vanishing flow when $\partial\Omega_2$ goes to infinity. Then the previous result can be applied to prove that in the two-dimensional case there are no well-behaved solutions for the flow past a body according to the linearized Boltzmann equation. We remark that Ukai and Asano[19] prove their existence theorem in a space of any dimension d, provided $d \geq 3$.

The result just discussed is well known in the theory of the Stokes equations[20], where it is known under the name of *Stokes paradox*. Here, following Ref. 9, we have extended it to the linearized Boltzmann equation.

In order to avoid a vanishing entropy flow on a large surface, we must allow for a logarithmically diverging bulk velocity. This would have no meaning, if we were solving exact equations; because of the linearization, however, we must consider whether the latter is permitted at large distances. The answer to this question is obviously negative, because at distances much larger than ℓ/M the linearization breaks down (the perturbation becomes singular[9]). The treatment of this aspect of the problem is outside the scope of the book.

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Chapter 7

Rarefied Lubrication in Mems

7.1 Introductory Remarks

The presence of a fluid film is known to reduce the sliding friction between solid objects. Although one usually thinks of a liquid (typically, oil), the case of a gas lubricant (typically, air) is also very important in several applications. Sometimes, problems of gas lubrication are not so obvious, because air is so easily available that one tends to disregard its presence. As technology expands and the size of components becomes smaller and smaller, the role of rarefied gases as lubricants becomes increasingly important. A typical example is provided by modern computers: the read/write head must be as close as possible to a rotating disk, and the air in between has accordingly a thickness of the order of a mean free path.

In lubrication theory, the thickness of the gas layer is extremely small compared with its lateral dimensions. Properly handled, this observation can be used to eliminate from the equations the dependence upon one of the three space variables. This possibility was exploited a long time ago by the famous hydrodynamicist Osborne Reynolds to integrate the mass balance equation across the layer and to use the linearized Navier–Stokes equation for momentum balance to evaluate the quantities appearing as integrands. Fortunately, Reynolds's argument can be extended to rarefied gases; the only difference is that the linearized Boltzmann equation must now be used to evaluate the averaged velocity components in the mass balance equation.

From a very superficial consideration of the matter one might expect that the main problem of lubrication theory is to predict the friction which results from a given configuration of solid objects. However, a little more reflection reveals that the real problem is quite different. Lubricating layers are usually found between two solid bodies which are acted upon by forces (such as gravity) tending to push them together. To carry this load, the gas layer must develop normal stresses, largely dominated by pressure. Thus the first task of lubrication theory is to predict the pressure distribution and from it the load-carrying capacity. Thus we must relate the velocity components to the pressure gradients and to the motion of the solid surfaces bounding the gas layer. Since the variations of thickness are very slow, this result is obtained by solving highly idealized problems between parallel plates, such as plane Couette and Poiseuille flows, which have been considered in the previous chapter. Thus these problems, far from being didactic exercises, play a very important role in applications of enormous practical importance.

7.2 The Modified Reynolds Equation

The starting point to obtain the rarefied version of the Reynolds equation for lubrication is the mass balance equation, a consequence of the Boltzmann equation that we considered in Chapter 1 (Eq. (1.6.18)). This equation is considerably simplified by the fact that the variations of density do not show up for slow motion in the steady flow case, which is the most important in applications and we shall consider henceforth. Thus we replace (Eq. (1.6.18) by

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \tag{7.2.1}$$

where the three velocity components are denoted by u, v, w.

Let us consider a layer of gas between two walls located at $z = 0$ and $z = D(x, y)$; the lower wall moves in its own plane (see Fig. 7.1, where, for simplicity, the z-direction has been suppressed). Let us integrate Eq. (7.2.1) across the layer to obtain

$$\int_0^D \frac{\partial u}{\partial x} dz + \int_0^D \frac{\partial v}{\partial y} dz + w(D) - w(0) = 0. \tag{7.2.2}$$

The normal velocity component vanishes at $z = 0$ and $z = D$. This gives

$$w = 0 \text{ at } z = 0 \text{ and } w = u\frac{\partial D}{\partial x} + v\frac{\partial D}{\partial y} \text{ at } z = D \tag{7.2.3}$$

and Eq. (7.2.2) becomes

$$\int_0^D \frac{\partial u}{\partial x} dz + \int_0^D \frac{\partial v}{\partial y} dz + \left[u\frac{\partial D}{\partial x} + v\frac{\partial D}{\partial y}\right]_{z=D} = 0, \tag{7.2.4}$$

which easily simplifies to

$$\frac{\partial}{\partial x}\int_0^D u dz + \frac{\partial}{\partial y}\int_0^D v dz = 0. \tag{7.2.5}$$

Since the problem is linear and the pressure gradient is assumed to be constant across the layer, each component u, v is proportional to the sum of the velocities given by a Poiseuille flow with pressure gradient dp/dx, dp/dy respectively and a

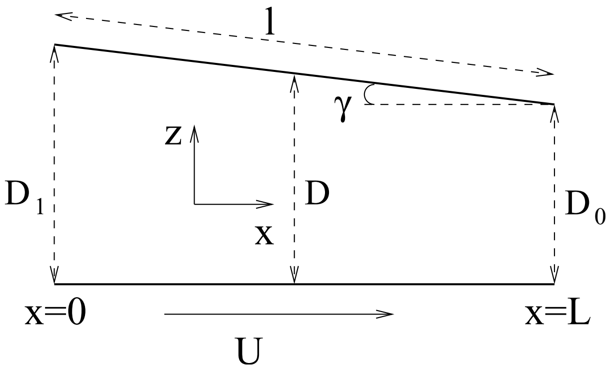

Figure 7.1: Geometry of a slider bearing.

Couette flow with the lower wall moving with velocity components U and V. We refer to Fig. 7.1 where, for simplicity, the y-axis has been suppressed.

In the case of Couette flow the evaluation of the integral:

$$F_C^{(1)} = \int_0^D u_C dz \tag{7.2.6}$$

is easy, if the walls are assumed to be identical. In fact, in this situation the profile is antisymmetric with respect to the midpoint and $u_C = U/2 + q(z - D/2)$ where $q(z)$ is an odd function; then

$$F_C^{(1)} = \frac{UD}{2} + \int_{-\frac{D}{2}}^{\frac{D}{2}} q(z)dz = \frac{UD}{2}. \tag{7.2.7}$$

Similarly

$$F_C^{(2)} = \int_0^D v_C dz = \frac{VD}{2}. \tag{7.2.8}$$

The behavior of the flow rate for plane Poiseuille flow is much more complicated and is given by

$$F_P^{(1)} = \int_0^D u_P dz = -\frac{1}{\rho_0\sqrt{2RT_0}}\frac{\partial p}{\partial x}D^2 Q(\delta),$$

$$F_P^{(2)} = \int_0^D v_P dz = -\frac{1}{\rho_0\sqrt{2RT_0}}\frac{\partial p}{\partial y}D^2 Q(\delta) \tag{7.2.9}$$

where δ is an inverse Knudsen number, the ratio between the distance and the (unperturbed) mean free path,

$$\delta = \frac{pD}{\mu\sqrt{2RT}}$$

and $Q(\delta)$ is the nondimensional flow rate which can be obtained by solving the problem of plane Poiseuille flow (see Section 5.6). Thus the modified Reynolds equation reads as

$$\frac{\partial}{\partial x}\left[\frac{\partial p}{\partial x}D^2Q(\delta)\right]+\frac{\partial}{\partial y}\left[\frac{\partial p}{\partial y}D^2Q(\delta)\right]=\rho_0\sqrt{2RT_0}\left[\frac{U}{2}\frac{\partial D}{\partial x}+\frac{V}{2}\frac{\partial D}{\partial y}\right]. \tag{7.2.10}$$

Given $D = D(x, y)$, this is an (elliptic) partial differential equation for p which must be solved for an assigned value of p (usually constant) at the boundary.

If, with $V = 0$, the length-to-breadth ratio is very large and if the leading and trailing edges of the floating body are straight, the side leakage may be negligible; then one can neglect the derivatives with respect to y and obtain an ordinary differential equation:

$$\frac{d}{dx}\left[\frac{dp}{dx}D^2Q(\delta)\right]=\rho_0\sqrt{2RT_0}\left[\frac{U}{2}\frac{dD}{dx}\right]. \tag{7.2.11}$$

This equation can be easily solved; in fact a first integral is

$$\frac{dp}{dx}D^2Q(\delta)=\rho_0\sqrt{2RT_0}\frac{U}{2}D+C, \tag{7.2.12}$$

where C is a constant of integration. A further integration gives

$$p=p_0+\rho_0\sqrt{2RT_0}\frac{U}{2}\int_0^x\frac{dx}{DQ(\delta)}+C\int_0^x\frac{dx}{D^2Q(\delta)}$$

where p_0 is another integration constant (the pressure at $x = 0$). If $0 \leq x \leq L$ and $p = p_0$ at $x = L$ as well, then

$$C=-\frac{\rho_0\sqrt{2RT_0}\frac{U}{2}\int_0^L\frac{dx}{DQ(\delta)}}{\int_0^L\frac{dx}{D^2Q(\delta)}}.$$

We have assumed so far that the linearization assumption holds everywhere. It may turn out, however, that the pressure undergoes a significant change. In this case, one can still utilize the linearized Boltzmann equation to compute the local flow rate, but one should use the local pressure p throughout, rather than the unperturbed pressure p_0. The modified Reynolds equation then reads as follows:

$$\frac{\partial}{\partial x}\left[\frac{D^2Q(\delta)}{\sqrt{2RT}}\frac{\partial p}{\partial x}\right]+\frac{\partial}{\partial y}\left[\frac{D^2Q(\delta)}{\sqrt{2RT}}\frac{\partial p}{\partial y}\right]=\frac{1}{2}\left[U\frac{\partial(\rho D)}{\partial x}+V\frac{\partial(\rho D)}{\partial y}\right]. \tag{7.2.13}$$

In the continuum limit we have

$$Q(\delta)=\frac{1}{6}\frac{pD}{\mu\sqrt{2RT}}$$

and Eq. (7.2.9) becomes

$$\frac{\partial}{\partial x}\left[\frac{\rho D^3}{\mu}\frac{\partial p}{\partial x}\right]+\frac{\partial}{\partial y}\left[\frac{\rho D^3}{\mu}\frac{\partial p}{\partial y}\right]=6\left[U\frac{\partial(\rho D)}{\partial x}+V\frac{\partial(\rho D)}{\partial y}\right] \tag{7.2.14}$$

which is essentially the equation originally given by Reynolds[15].

7.3 The Reynolds Equation and the Flow in a Microchannel

Micromachinery fabrication techniques have become more and more mature in the last ten years. In particular, micro-electro-mechanical systems (MEMS) developed rapidly and found many applications in microelectronics, medicine, biology, optics, aerospace and other high technology fields. Both experimental and computational efforts have been undertaken to understand the specific features of microscale flows. A basic constituent of the MEMS devices is the microchannel , the region between two parallel plates that can reveal many specific features of the low speed internal flows in microdevices. Typically the first devices were integrated micro-channel/pressure sensor systems. The Knudsen number at the outlet of the channel at room conditions is 0.05 for nitrogen, and even higher for helium; hence the flow is surely beyond the slip flow regime. The pressure distribution along the channel and the flow rates across these channels are found to deviate from the linear distribution of the Poiseuille flow. Monte Carlo methods were used to simulate microchannel flows but they meet with excessively high demands of storage and computation time. The gradual regulation of the inlet and outlet boundary conditions of the channel seems to be tremendously difficult for DSMC in solving the long channel flows. In fact the typical DSMC simulation of the micro channel flow is limited to high speeds. Recently, the so-called information preservation (IP) method was proposed[8,9]; it uses a conservative scheme and a super-relaxation technique, with results in excellent agreement with experimental data. As an example, Jiang, Shen and Fan[12] solved the thin film air bearing problem by the IP method. Fig. 7.2 shows the comparison of the pressure distributions for the case of a channel length $L = 1000\mu m$ calculated by the IP method and of the generalized Reynolds equation.

However, the methods discussed in this book indicate that kinetic theory of MEMS does not require heavy computational tools. The generalized Reynolds equation can be used to calculate the gas film lubrication problem provided that the flow rate of Poiseuille flow is calculated from the linearized Boltzmann equation. The microchannel flow problem is particularly simple because the generalized Reynolds equation degenerates into a very simple ordinary differential equation[14]. In this case, in fact, the upper plate is parallel to the lower one, which is at rest. Thus the right-hand side of Eq. (7.2.12) vanishes, and D is a constant. Further no dependence on y occurs. Hence the generalized Reynolds equation for a microchannel becomes

$$\frac{d}{dx}\left[\frac{Q(\delta)}{\sqrt{2RT}}\frac{dp}{dx}\right] = 0. \tag{7.3.1}$$

The values of the pressure p on the inlet and outlet of the channel are to be specified to solve the problem. For the case of diffuse reflection, $Q(\delta)$ is available from databases and there is even a fitting formula approximation by Robert recorded in Ref. 1:

$$Q(\delta) = \frac{1}{6}\delta + A + \frac{1}{\sqrt{\pi}}\log(1 + \frac{B}{\delta}) \tag{7.3.2}$$

where $A = 1.318889$ and $B = 0.387361$. Thus assuming temperature to be constant, we have

$$\left[\frac{1}{6}\delta + A + \frac{1}{\sqrt{\pi}}\log(1 + \frac{B}{\delta})\right]\frac{dp}{dx} = C \tag{7.3.3}$$

where C is a constant to be determined from the boundary conditions.

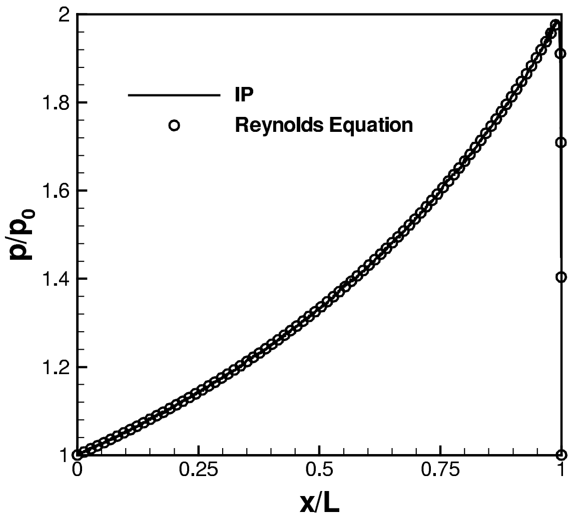

Figure 7.2: Pressure distribution in the disc driver bearing for Kn=1.25, $L = 1000\mu m$; comparison of the results from IP and the generalized Reynolds equation[12]. (Courtesy of C. Shen, Fig. 8.23 of Ref. 18.)

Although very simple, the procedure illustrated above seems to have been considered only very recently by C. Shen[16], who illustrated the use of the degenerated Reynolds equation in solving the microchannel problem. Taking the experimental data of References 14 and 19, he obtained by integration the results presented in Figs. 7.3 and 7.4. The agreement between the results from the Reynolds equation and the results from IP is excellent. The experimental data agree with the above two methods within the limit of experimental accuracy. Other results and comparisons of the integration of the degenerated Reynolds equation with the DSMC and IP results are shown in Fig. 7.5 and Fig. 7.6.

Also shown in the figures are the results from the so-called Lattice Boltzmann method[13]. From the comparison it is seen that the DSMC method, the IP

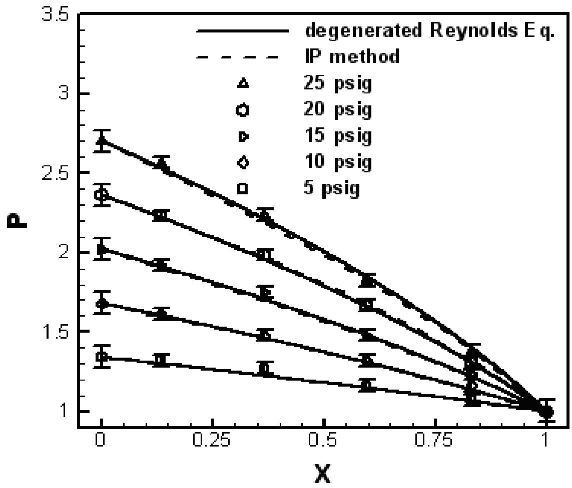

Figure 7.3: The pressure distribution in a $1.2 \times 40 \times 3000 \mu m^3$ microchannel for nitrogen. Comparison[16] of the degenerated Reynolds equation (7.3.1) (solid lines), the IP method (dashed lines) and the experimental data[14]. (Courtesy of C. Shen, Fig. 8.24 of Ref. 18.)

method and the degenerated Reynolds equation yield almost identical pressure distribution, but the LBM results are quite different from the DSMC and IP results and also from calculation of the degenerated Reynolds equation, so the version of Lattice Boltzmann method employed in Reference 13 is not feasible for simulating microchannel flows in the transitional regime. For a detailed examination of feasibility of the Lattice Boltzmann method in simulating transitional regime microchannel flows the reader is referred to Reference 17.

The calculation of the flow rate of Poiseuille flow based on the methods of kinetic theory is of great interest in many practical applications; a further discussion is given in the next section.

7.4 The Poiseuille-Couette Problem

Following Ref. 4, let us consider again two plates separated by a distance D and a gas flowing parallel to them, in the x direction, due to a pressure gradient. The lower boundary ($z = -D/2$) moves to the right with velocity U, while the upper boundary ($z = D/2$) is fixed. Both boundaries are held at a constant temperature T_o. However, at variance with our previous discussions, we assume the gas-surface interaction to be different at the wall.

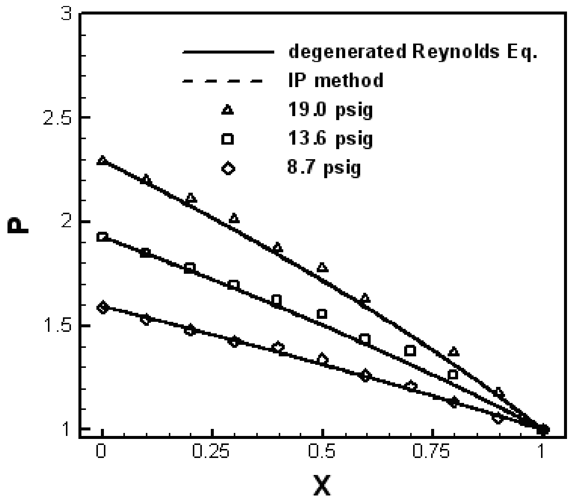

Figure 7.4: The pressure distribution in a $1.2 \times 40 \times 4000 \mu m^3$ microchannel for helium. Comparison[16] of the degenerated Reynolds equation (7.3.1) (solid line), the (dashed lines, lines, note that the solid lines and the dashed lines almost coincide) and the experimental data[19]. (Courtesy of C. Shen, Fig. 8.25 of Ref. 18.)

As usual, if the pressure gradient and the velocity U are taken to be small, it can be assumed that the Boltzmann equation can be linearized about a Maxwellian. If we assume the linearized BGK model for the collision operator, the Boltzmann equation reads

$$\frac{1}{2}k + \zeta \frac{\partial Z}{\partial z} = \frac{1}{\ell}\left[\pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-c_{z_1}^2} Z(z, c_{z_1})\, dc_{z_1} - Z(z,\zeta)\right] \tag{7.4.1}$$

where by definition

$$Z(z,\zeta) = \pi^{-1} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-c_x^2 - c_y^2} c_x h(z, \mathbf{c})\, dc_x\, dc_y,$$

$$k = \frac{1}{p}\frac{\partial p}{\partial x} = \frac{1}{\rho}\frac{\partial \rho}{\partial x},$$

with p and ρ being the gas pressure and density, respectively, and ℓ the mean free path. Consequently, the bulk velocity of the gas is given by

$$q(z) = \pi^{-\frac{1}{2}} \int_{-\infty}^{+\infty} e^{-c_{z_1}^2} Z(z, c_{z_1})\, dc_{z_1}. \tag{7.4.2}$$

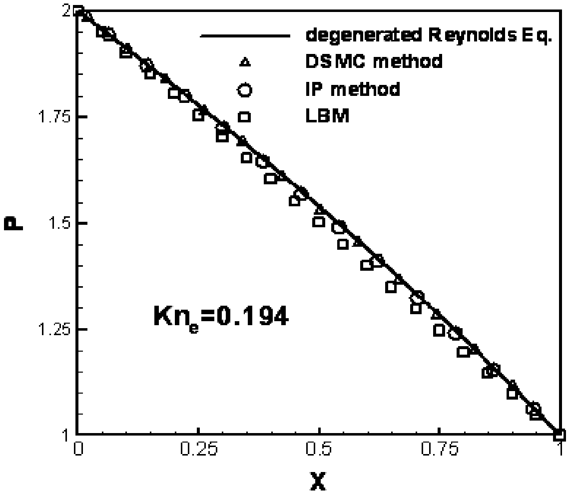

Figure 7.5: Pressure distribution in a microchannel with Kn=0.194 at outlet ($D/L = 100$). Comparison[16] of the degenerated Reynolds equation, DSMC, IP methods and the LBM method. (Courtesy of C. Shen, Fig. 8.26 of Ref. 18.)

From Eq. (7.4.1) we obtain the integral equation

$$\begin{aligned} Z(z,\zeta) = {} & \exp(-(z+\frac{D}{2}\mathrm{sgn}\zeta)/(\zeta\ell))Z(-\frac{D}{2}\mathrm{sgn}\zeta,\zeta) \\ & + \int_{-\frac{D}{2}sgn\zeta}^{z} \exp\left(\frac{-|z-t|}{|\zeta|\ell}\right)[q(t)-k\ell/2]/(\zeta\ell)\,dt, \end{aligned} \tag{7.4.3}$$

with the values at the boundary, $Z(-\frac{D}{2}\mathrm{sgn}\zeta,\zeta)$, depending on the model of boundary conditions chosen. In the following, we will consider the Maxwell boundary conditions and consider two walls having different physical properties, i.e., with two accommodation coefficients (α_1,α_2). In this case, the boundary conditions can be written as

$$Z^+(D/2,\zeta) = (1-\alpha_1)Z^-(D/2,-\zeta),$$

$$Z^+(-D/2,\zeta) = \alpha_2 U + (1-\alpha_2)Z^-(-D/2,-\zeta),$$

where U is expressed in units of $(2RT_o)^{1/2}$; $Z^-(-D/2,\zeta)$, $Z^-(D/2,\zeta)$ are the distribution functions of the molecules impinging upon the walls and $Z^+(-D/2,\zeta)$, $Z^+(D/2,\zeta)$ the distribution functions of the molecules reemerging from the same walls.

Once the function at the boundary, $Z(-\frac{D}{2}\mathrm{sgn}\zeta,\zeta)$, has been evaluated following the analytical procedure reported in Refs. 7 and 5 , the substitution of

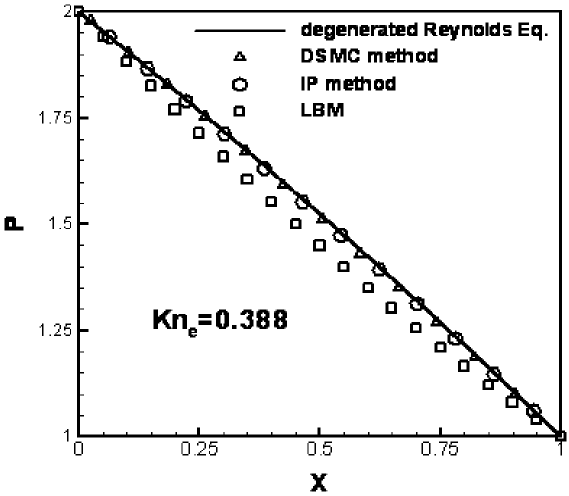

Figure 7.6: Pressure distribution in a microchannel with Kn=0.388 at outlet ($D/L = 100$). Comparison[16] of the degenerated Reynolds equation, DSMC, IP methods and the LBM method. (Courtesy of C. Shen, Fig. 8.27 of Ref. 18.)

the integral formula (7.4.3) in the definition (7.4.2) of $q(z)$ gives the following expression for the bulk velocity of the gas:

$$q(z) = \frac{1}{2}k\ell[1 - \psi_p(u)] + U\psi_c(u). \tag{7.4.4}$$

Eq. (7.4.4) shows that the gas velocity is induced by the superposition of two distinct effects. The gas moves by an imposed pressure gradient (Poiseuille flow) and by the shear driven flow due to the motion of the bottom surface (Couette flow). The nondimensional functions $\psi_p(u)$ and $\psi_c(u)$, giving the Poiseuille and Couette contributions, respectively, satisfy the following integral equations:

$$\begin{aligned}
\psi_p(u) = \; & 1 + \frac{1}{\sqrt{\pi}} \int_{-\delta/2}^{\delta/2} dw \psi_p(w) \Big\{ (1-\alpha_1) S_{-1}(\delta - u - w) \\
& + (1-\alpha_2) S_{-1}(\delta + u + w) \\
& + (1-\alpha_1)(1-\alpha_2)[S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] \\
& + T_{-1}(|u-w|) \Big\},
\end{aligned} \tag{7.4.5}$$

$$\begin{aligned}
\psi_c(u) = \; & \frac{\alpha_2}{\sqrt{\pi}}\Big[T_o(\delta/2+u) + (1-\alpha_1)S_o(3/2\delta - u) \\
& +(1-\alpha_1)(1-\alpha_2)S_o(5/2\delta + u)\Big] \\
& +\frac{1}{\sqrt{\pi}}\int_{-\delta/2}^{\delta/2} dw\psi_c(w)\Big\{(1-\alpha_1)S_{-1}(\delta - u - w) \\
& +(1-\alpha_2)S_{-1}(\delta + u + w) \\
& +(1-\alpha_1)(1-\alpha_2)[S_{-1}(2\delta - u + w) + S_{-1}(2\delta + u - w)] \\
& +T_{-1}(|u-w|)\Big\},
\end{aligned} \tag{7.4.6}$$

where $T_n(x)$ is the Abramowitz function defined by

$$T_n(x) = \int_0^{+\infty} t^n \exp(-t^2 - x/t)\, dt.$$

$S_n(x)$ is a generalized Abramowitz function defined by

$$S_n(x, \delta, \alpha_1, \alpha_2) = \int_0^{+\infty} \frac{t^n \exp(-t^2 - x/t)}{1-(1-\alpha_1)(1-\alpha_2)\exp(-2\delta/t)}\, dt$$

and the following nondimensional variables have been introduced:

$$\delta = D/\ell, \qquad w = t/\ell, \qquad u = z/\ell.$$

Using Eq. (7.4.4), the flow rate (per unit time through unit thickness) defined by[2]

$$F = \rho \int_{-D/2}^{D/2} q(z) dz \tag{7.4.7}$$

can be expressed as the sum of the Poiseuille flow (F_p) and the Couette flow (F_c) as follows:

$$F = F_p + F_c = -\frac{\partial p}{\partial x} D^2 Q_p(\delta, \alpha_1, \alpha_2) + \frac{\rho U D}{2} Q_c(\delta, \alpha_1, \alpha_2) \tag{7.4.8}$$

where

$$Q_p(\delta, \alpha_1, \alpha_2) = -\frac{1}{\delta} + \frac{1}{\delta^2}\int_{-\delta/2}^{\delta/2} \psi_p(u) du,$$

$$Q_c(\delta, \alpha_1, \alpha_2) = \frac{2}{\delta}\int_{-\delta/2}^{\delta/2} \psi_c(u) du$$

are the nondimensional volume flow rates.

7.5 The Generalized Reynolds Equation for Unequal Walls

One can easily extend the generalized Reynolds equation to the case of unequal walls:

$$\frac{d}{dx}\left(\frac{dp}{dx}D^2Q_p(\delta,\alpha_1,\alpha_2)-\frac{\rho UD}{2}Q_c(\delta,\alpha_1,\alpha_2)\right)=0. \tag{7.5.1}$$

For the purpose of a direct comparison with the classical Reynolds equation (7.2.12), let us introduce the Poiseuille relative flow rate[10,11]

$$\tilde{Q}_p(\delta,\alpha_1,\alpha_2)=\frac{Q_p(\delta,\alpha_1,\alpha_2)}{Q_{con}} \tag{7.5.2}$$

where $Q_{con}=\delta/6$. Furthermore, the rarefaction parameter δ can be expressed as $\delta=\delta_o PH$, where δ_o is the characteristic inverse Knudsen number defined by the minimum film thickness, D_o, and the ambient pressure p_o as

$$\delta_o=\frac{p_oD_o}{\mu\sqrt{2RT_o}}.$$

Finally, assuming that the heat generation in the gas is very small, so that an isothermal process can be considered, the nondimensional generalized Reynolds equation reads

$$\frac{d}{dX}\left(\tilde{Q}_p(\delta_oPH,\alpha_1,\alpha_2)PH^3\frac{dP}{dX}-Q_c(\delta_oPH,\alpha_1,\alpha_2)\Lambda PH\right)=0. \tag{7.5.3}$$

Here the bearing number Λ is defined as

$$\Lambda=\frac{6\mu Ul}{p_oD_o^2} \tag{7.5.4}$$

where μ is the viscosity coefficient. If the two walls are identical ($\alpha_1=\alpha_2=\alpha$), the Couette flow rate is independent of the Knudsen number regardless of the value of the accommodation coefficient α and Eq. (7.5.3) reduces to the generalized Reynolds equation introduced by Fukui and Kaneko[10,11].

Writing the nondimensional film thickness H in terms of the longitudinal coordinate X,

$$H=\frac{D_1}{D_o}-\frac{l}{L}\left(\frac{D_1}{D_o}-1\right)X \tag{7.5.5}$$

such that

$$\frac{dP}{dX}=-\frac{l}{L}\left(\frac{D_1}{D_o}-1\right)\frac{dP}{dH},$$

Eq. (7.5.3) can be immediately integrated to give

$$\frac{l}{L}\left(\frac{D_1}{D_o}-1\right)\tilde{Q}_p(\delta_oPH,\alpha_1,\alpha_2)PH^3\frac{dP}{dH}+Q_c(\delta_oPH,\alpha_1,\alpha_2)\Lambda PH=K_1 \tag{7.5.6}$$

where K_1 is a constant of integration. The substitution of

$$PH = \zeta \tag{7.5.7}$$

in Eq. (7.5.6) gives

$$\frac{d\zeta}{dH} = \frac{\zeta}{H} - \frac{[Q_c(\delta_o\zeta, \alpha_1, \alpha_2)\Lambda\zeta - K_1]}{l/L(D_1/D_o - 1)\tilde{Q}_p(\delta_o\zeta, \alpha_1, \alpha_2)H\zeta}. \tag{7.5.8}$$

Eq. (7.5.8) can be solved numerically using relaxation methods. To apply this numerical scheme, the differential equations have to be replaced by finite-difference equations on a point mesh. The solution of the resulting set of equations is determined by starting with a guess and improving it iteratively using Newton's method. The Poiseuille flow rate coefficient $Q_p(\delta, \alpha_1, \alpha_2)$ has been evaluated by means of the numerical method described in Ref. 7 and the variational technique for the integrodifferential form of the Boltzmann equation based on the BGK model. In order to compute the Couette flow rate $Q_c(\delta, \alpha_1, \alpha_2)$ one can solve numerically Eq. (7.4.6), extending a finite difference technique first introduced by Cercignani and Daneri[2].

Once $\zeta(H)$ has been numerically evaluated on a grid that spans the domain of interest, Eqs. (7.5.5) and (7.5.7) give the pressure field in the gas film as a function of X. Furthermore, a prediction of the vertical force acting on the upper surface of the slider bearing, crucial for practical design, may be obtained from the load carrying capacity W, defined as

$$W = \frac{l}{L}\int_0^{L/l} (P - 1)\, dX. \tag{7.5.9}$$

In order to investigate the effects of the rarefaction parameter δ_o and the bearing number Λ on the basic lubrication characteristics (pressure distribution and load carrying capacity), the parameters describing the gas film geometric configuration were fixed at the following values: $D_1/D_o = 2$, $L/D_o = 100$. Figures 7.7 and 7.8 show the pressure field as a function of the longitudinal coordinate X at three different bearing numbers: $\Lambda = 10, 50, 200$. To assess the influence of the boundary conditions, the profiles corresponding to different accommodation coefficients (for bounding walls supposed physically identical) are drawn in Figs. 7.7 and 7.8.

Looking at the pictures, one sees that the pressure distribution in the gas film increases with increasing Λ. Furthermore, at fixed bearing number, the pressure field reduces by increasing the fraction of gas molecules specularly reflected by the walls. Figs. 7.9 and 7.10 report the pressure profiles for the same parameters as in Figs. 7.7 and 7.8, except that now the two bounding plates are allowed to re-emit the impinging gas molecules differently, so that two accommodation coefficients can be defined. We keep the accommodation coefficient of the upper wall (α_1) fixed and vary the other one (α_2).

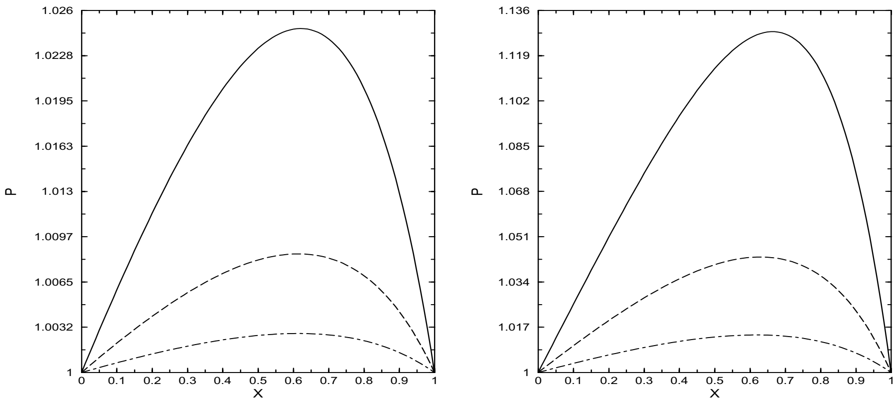

Figure 7.7: Pressure profile for $\delta_o = 0.5$. The line styles indicate $\alpha = 0.8$ (solid), $\alpha = 0.3$ (dashed), and $\alpha = 0.1$ (dot dashed). The bearing number Λ is 10 (left) and 50 (right).

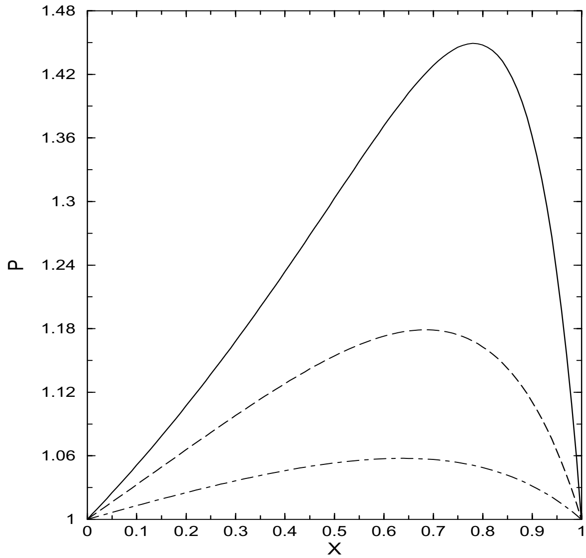

Figure 7.8: Pressure profile for $\delta_o = 0.5$. The line styles indicate $\alpha = 0.8$ (solid), $\alpha = 0.3$ (dashed), and $\alpha = 0.1$ (dot dashed). The bearing number Λ is 200.

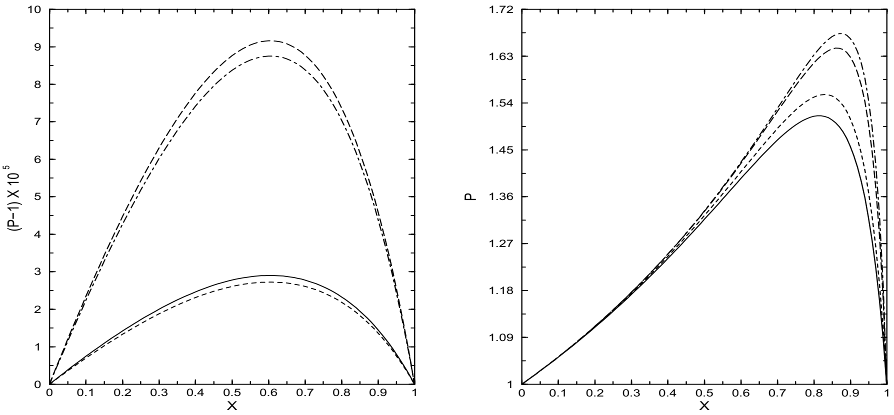

Figure 7.9: Pressure profile for $\delta_o = 0.5$. The line styles indicate $\alpha_1 = 0.5$ $\alpha_2 = 0.8$ (solid), $\alpha_1 = 0.5$ $\alpha_2 = 0.3$ (dashed), and $\alpha_1 = 0.5$ $\alpha_2 = 0.1$ (dot dashed). The bearing number Λ is 10 (left) and 50 (right).

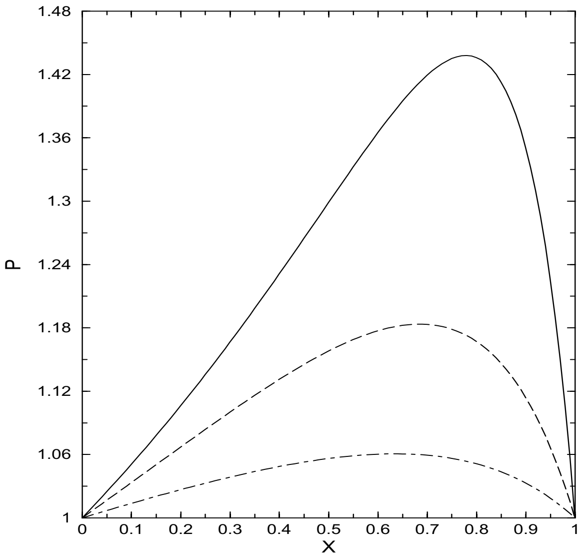

Figure 7.10: Pressure profile for $\delta_o = 0.5$. The line styles indicate $\alpha_1 = 0.5$ $\alpha_2 = 0.8$ (solid), $\alpha_1 = 0.5$ $\alpha_2 = 0.3$ (dashed), and $\alpha_1 = 0.5$ $\alpha_2 = 0.1$ (dot dashed). The bearing number Λ is 200.

A comparison with Figs. 7.7 and 7.8 shows that, for every Λ, the pressure distribution significantly depends on α_2 and only weakly on α_1. This picture remains true at different Knudsen numbers progressing from free molecular, through transitional, to continuum regions.

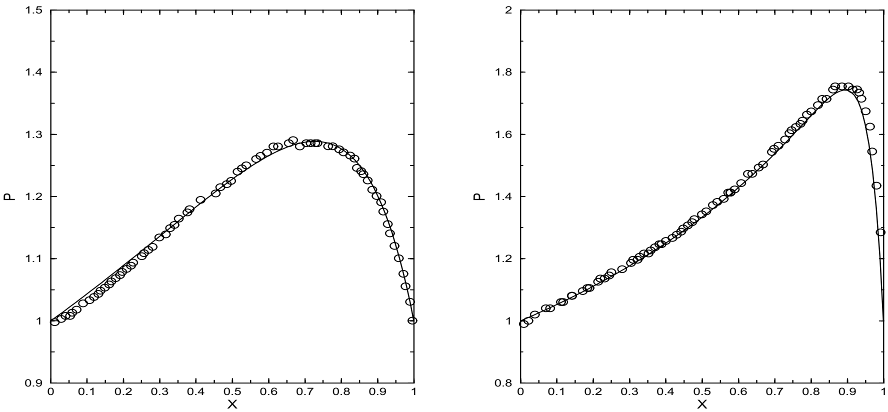

Figure 7.11: Pressure profile versus X. Comparison between the results obtained with the modified Reynolds equation (solid line) and DSMC data [1] (open circles). The parameters are: $\delta_o = 0.7$, $\Lambda = 61.6$, $\alpha = 1$ (left); $\delta_o = 0.2$, $\Lambda = 1264$, $\alpha = 1$ (right).

It is worth noting that, when Λ increases, the Couette contribution to the lubrication flow rate becomes dominant compared with the Poiseuille flow. Therefore, if the two walls are identical, the influence of the Knudsen number on the load carrying capacity decreases as Λ increases, since Q_c is independent of δ and α. On the contrary, if the two walls have a different physical structure the load carrying capacity shows a dependence on both the Knudsen number and the accommodation coefficients α_1, α_2. For the validation of the code, the results obtained with the modified Reynolds equation have been compared with the results from DSMC (Direct Simulation Monte Carlo) simulations published by Alexander et al.[1] in the case of Maxwell's boundary conditions on two physically identical walls (see Figs. 7.11 and 7.12).

7.6 Concluding remarks

In this final chapter we have described some recent applications of the methods of kinetic theory to the slow rarefied flows which occur in MEMS. This area is, however, in rapid expansion. We should expect new results for geometries more complicated than those considered here, which cannot, even locally, be approximated by parallel plates. In this context, a method introduced in the late 1960s[3,4]

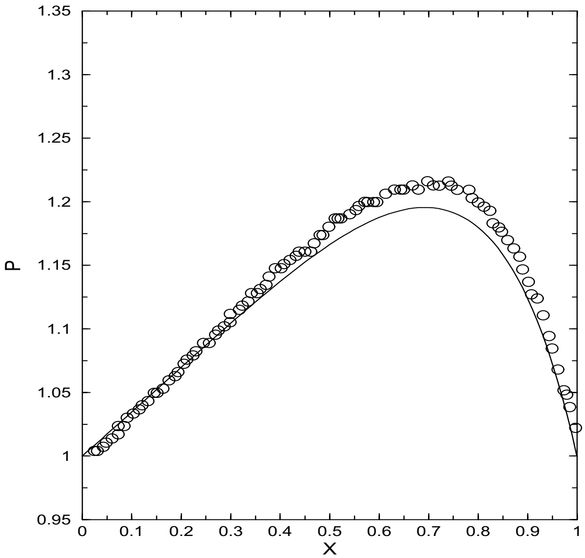

Figure 7.12: Pressure profile versus X. Comparison between the results obtained with the modified Reynolds equation (solid line)and DSMC data[1] (open circles). The parameters are: $\delta_o = 0.7$, $\Lambda = 61.6$, $\alpha = 0.7$.

to supply appropriate boundary conditions to permit computations of flows in the transition regime by means of the Navier–Stokes equations might turn out to be useful.

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