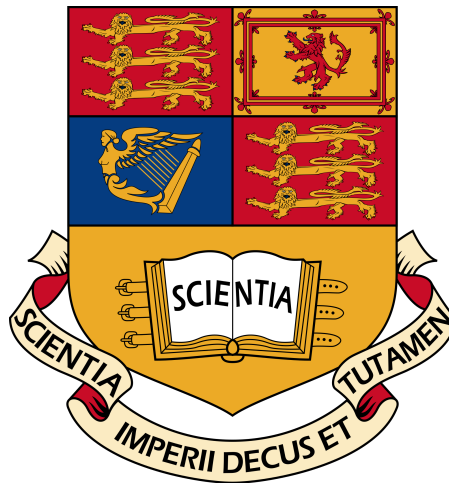


Hilbert's Sixth Problem

From Micro to Macroscopic Descriptions



Maria del Valle Varo

Supervisor: Dr. Jonathan Ben-Artzi

Imperial College London

Summer project part of the
Undergraduate Research Opportunities Programme

London 2016

“The second law of thermodynamics can be explained mechanically by
the unprovable assumption that...
the universe is an improbable state.”

— *Letter of Boltzmann to Zermelo* [1]

Contents

1	Introduction	1
2	Microscopic	3
2.1	Billiard Balls	3
2.2	Liouville's Theorem	5
2.3	Comment	6
3	Kinetic Theory	7
3.1	Boltzmann Equation	7
3.2	Conservation Laws	9
3.3	Equilibrium States	10
3.4	Boltzmann's H theorem	11
4	Incompressible Navier-Stokes	13
5	The Bridge:	
	from microscopic to mesoscopic	17
5.1	BBGKY Hierarchy	17
6	Conclusion	20

1

Introduction

The 6th Problem differs significantly from the other 22 Hilbert's problems [2]. The title of the problem itself is mysterious: "Mathematical treatment of the axioms of physics". Physics, in its essence, is a special activity for the creation, validation and destruction of theories for real-world phenomena, where "We are trying to prove ourselves wrong as quickly as possible, because only in that way can we find progress" [3]. There exist no mathematical tools to formalise relations between Theory and Reality in live Physics. Therefore the 6th Problem may be viewed as a tremendous challenge in deep study of ideas of physical reality in order to replace vague philosophy by a new logical and mathematical discipline. Some research in quantum observation theory and related topics can be viewed as steps in that direction, but it seems that at present we are far from an understanding of the most logical and mathematical problems here. The first explanation of the 6th Problem given by Hilbert reduced the level of challenge and made the problem more tractable: "The investigations on the foundations of geometry suggest the problem: To treat in the same manner, by means of axioms, those physical sciences in which mathematics plays an important part; in the first rank are the theory of probabilities and mechanics". This is definitely "a programmatic call" [?] for the axiomatising of the formal parts of existent physical theories and no new universal logical framework for the representation of reality is necessary. In this context, the axiomatic approach is a tool for the retrospective analysis of well-established and elaborated physical theories and not for live physics.

For the general statements of the 6th Problem it seems unclear now how to formulate criteria of solutions. In a further explanation Hilbert proposed two specific problems: (i) axiomatic treatment of probability with limit theorems for foundation of statistical physics and (ii) the rigorous theory of limiting processes "which lead from the atomistic view to the laws of motion of continua". For complete resolution

of these problems Hilbert has set no criteria either but some important parts of them have been already claimed as solved.

The way from the “atomistic view to the laws of motion of continua” is not so well formalised. It includes at least two steps: (i) from mechanics to kinetics (from Newton to Boltzmann) and (ii) from kinetics to mechanics and non-equilibrium thermodynamics of continua (from Boltzmann to Euler and Navier–Stokes–Fourier). The first part of the problem, the transition from the reversible-in-time equations of mechanics to irreversible kinetic equations, is still too far from a complete rigorous theory. The highest achievement here is the proof that hard spheres will follow the Boltzmann equation during a fraction of the collision time, starting from a non-correlated initial state, which is resembled in Lanford theorem [4]. The BBGKY hierarchy, which will be presented later, provides the general framework for this problem. For the systems close to global thermodynamic equilibrium the global in time estimates are available and the validity of the Boltzmann equation is proven recently in this limit for gas of hard spheres [5]. The second part, model reduction in dissipative systems, from kinetics to macroscopic dynamics, is ready for a mathematical treatment. Some limit theorems about this model reduction are already proven, and open questions can be presented in a rigorous mathematical form. In this project, we will present the current most basic models for the microscopic, mesoscopic and macroscopic description of fluids, and discuss briefly the mathematical bridges built between them so far, adding a final note about the question of how can we obtain time-asymmetric results from an apparently only time-symmetric (invariant) assumptions.

2

Microscopic

The history of Classical Mechanics goes back to the Greeks where Aristotle made first reference in his *On the Heavens*, to the relation between movements and forces. A long time passed until the fundamental principles of classical mechanics were laid down by Galileo and Newton in the 16th and 17th centuries [6]. Afterwards, around 50 years later, Leonhard Euler expanded Newton's Laws of motion from particles to rigid bodies with two additional laws. These laws, all together with Newton's laws, were later reformulated into the Lagrangian and the Hamiltonian formalism. The first is associated with configuration space, while the latter is the natural description for working in phase space [7]. This means, a point in configuration space represents configuration of the system, i.e. positions of the constituent particles. While a point in phase space represents state of the system, i.e. positions and velocities of the constituent particles together.

Hamiltonian mechanics became a very useful way of looking at classical mechanics later, and contributed to the formulation of statistical mechanics and quantum mechanics. By the end of the 20th century, classical mechanics stopped being an independent theory and became embedded in relativistic quantum mechanics[8].

2.1 Billiard Balls

Suppose we have N billiard balls. We will label each with i or j , where $i, j = 1, \dots, N$. They will have the same mass and their motion will follow Hamilton's equations, and this is what we shall call the Microscopic view (relativistic and quantum effects will not be considered in this project).

Taking the Hamiltonian to be of a general form[9]:

$$H = \frac{1}{2m} \sum_{i=1}^N \vec{p}_i^2 + \sum_{i=1}^N V(\vec{r}_i) + \sum_{i < j} U(\vec{r}_i - \vec{r}_j) \quad (2.1)$$

This Hamiltonian contains an external force $\vec{F} = -\nabla V$ that acts equally on all particles. There are also two-body interactions between particles, captured by the potential energy $U(\vec{r}_i - \vec{r}_j)$. We will also assume that the potential is short-ranged, meaning that $U(r) \approx 0$ for $r \gg \epsilon$, being ϵ the diameter of the billiard balls. The condition of $i < j$ is included such that we do not count the particles interactions twice. Hence, the Hamilton's equations are:

$$\frac{\partial H}{\partial \vec{x}} = -\frac{\partial \vec{p}}{\partial t} = \quad \text{and} \quad \frac{\partial H}{\partial \vec{p}} = \frac{\partial \vec{x}}{\partial t} \quad (2.2)$$

But because we are treating with a much simpler system (such as billiard balls), the Hamilton's equations can be simplified to:

$$\frac{dx_i}{dt} = v_i \quad \text{and} \quad \frac{dv_i}{dt} = 0 \quad (2.3)$$

Except at the times of collision, when the particle's velocity changes instantly and there is a discontinuity. A collision will occur when $|x_i - x_j| = \epsilon$. Defining the unitary vector such that:

$$\vec{n} = \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|}$$

A schematic sketch is done here to illustrate a collision between two balls. Ball 1 and 2 collide and depart with different velocities, which form a collision disc (figure of the right) which encapsulates the conservation laws presented below:

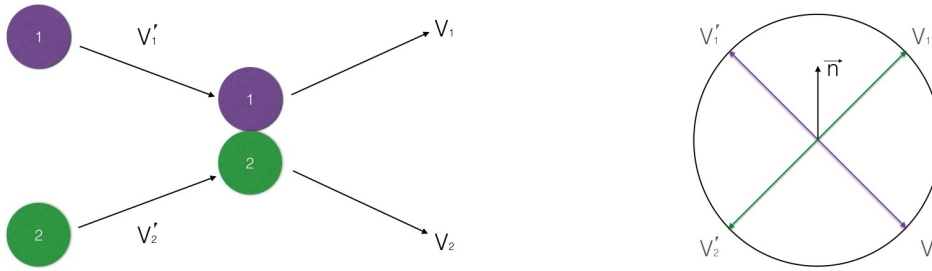


Figure 2.1: Where \vec{v}'_1 is the first ball initial velocity, \vec{v}'_2 second ball initial velocity and Where \vec{v}_1 and \vec{v}_2 their velocities after the collision respectively. And \vec{n} is the vector defined above.

With these equations and geometry principles, the first conservation laws can be

derived for a possible collision:

$$\begin{aligned}
\text{Conservation of energy:} \quad & |v_i|^2 + |v_j|^2 = |v'_i|^2 + |v'_j|^2 \\
\text{Conservation of momentum:} \quad & \vec{v}'_i + \vec{v}'_j = \vec{v}_i + \vec{v}_j \\
\text{Specular reflection:} \quad & \vec{v}_i = \vec{v}'_i - (\vec{v}'_i - \vec{v}'_j) \cdot \vec{n} \\
& \vec{v}_j = \vec{v}'_j - (\vec{v}'_j - \vec{v}'_i) \cdot \vec{n}
\end{aligned}$$

These conservation laws along with Hamilton's equations are sufficient to determine all possible trajectories and velocities of the particles at stake. An important remark, is that this is all a deterministic system, meaning that all the information is conserved and is comprised in the Hamiltonian.

2.2 Liouville's Theorem

One of the usefulness of using Hamiltonian formalism for classical mechanics is found in Liouville's Theorem. In Classical Mechanics, the complete state of a particle can be given by its spatial coordinates and momenta. For example in three dimensions, there are three spatial coordinates and three conjugate momenta. If we consider a six dimensional phase space, a point in that space represents the state of a particle. A particle will follow a determined path through phase space, that is, given the particles full state (a point in phase space), our equations of motion will yield the phase space location of the particle at any point in time. So particles follow determined paths through a six dimensional phase space.

Now we would like to discuss what will occur when the number of billiard balls N , tends to a very big number (of the order of Avogadro's number). This seems in principle rather complicated, since we would have N -coupled equations. This is the beginning of how Kinetic Theory evolved, which will be discussed later to arrive to the Boltzmann equation. For now, we will consider the most important feature of Liouville's theorem: the phase space distribution function[10] . This probability function in the vicinity of phase space (\vec{x}_i, \vec{p}_i) is:

$$\int dV f(\vec{x}_i, \vec{p}_i; t) = 1 \quad \text{with} \quad dV = \prod_{i=1}^N d^3x_i d^3p_i \quad (2.4)$$

The probability function contains all the information that there is about each particle at any point in time. This means that it must be conserved, and so it must obey the continuity equation in phase space which is:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{x}_i} (\dot{\vec{x}}_i f) + \frac{\partial}{\partial \vec{p}_i} \cdot (\dot{\vec{p}}_i f) = 0 \quad (2.5)$$

Making substitution with Hamilton's equations 2.2:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{x}_i} \cdot \frac{\partial H}{\partial \vec{p}_i} f - \frac{\partial}{\partial \vec{p}_i} \frac{\partial H}{\partial \vec{x}_i} f = 0 \quad (2.6)$$

This is the *Liouville's equation*. Nevertheless, it is convenient to introduce a certain formalism which enable one to write these equations briefly [11], namely the Poisson bracket formalism. If we have two functions say $A(r, s)$ and $B(r, s)$ which are depend on two variables r and s (independent of each other), then they have a Poisson bracket such that:

$$\{A, B\} = \frac{\partial A}{\partial r} \frac{\partial B}{\partial s} - \frac{\partial A}{\partial s} \frac{\partial B}{\partial r}$$

Equation 2.6 can thus written concisely in the Poisson bracket formalism:

$$\frac{\partial f}{\partial t} = \{H, f\} \quad (2.7)$$

The time-development of the f function is given then by the Poisson bracket of the function with the Hamiltonian. The system will be found in equilibrium when f is a function of the Hamiltonian, and hence they will commute [9]. The Liouville's equations lead inevitably to the Liouville's theorem which reads: "The distribution function is constant along any trajectory in phase space". This means: if you follow some region of phase space under Hamiltonian evolution, then its shape can change but its volume remains the same[12], which is also a statement of reversibility.

2.3 Comment

But what happens when N tends to infinity? The problem we are concerned with here is, if we have N particles that are govern by Newtonian laws, will we be able to predict their future motion only from classical mechanics? The answer to the question is: *yes, in principle*. If we have all the information for each ball and we have a good enough computer to calculate all the trajectories. In reality, this is something that is rather unrealistic (more due to the lack of information rather than the computational power), but that nevertheless is theoretically plausible. The BBGKY will give us some insight into how to proceed, in section 5.

3

Kinetic Theory

The kinetic theory of gases is the study of the microscopic behaviour of molecules and the interactions which lead to macroscopic relationships. The assumptions to arrive to the Kinetic Model are:

- Molecules obey Hamiltonian mechanics.
- No external force exists.
- Molecules undergo elastic collisions.
- Only binary collisions occur.

3.1 Boltzmann Equation

In 1872 Boltzmann started from the by the time accepted atomistic model and wrote a nonlinear transport equation for the one-particle distribution function [13]. The Boltzmann equation or Boltzmann transport equation describes the statistical behaviour of a thermodynamic system not in a state of equilibrium. The equation arises not by statistical analysis of all the individual positions and momenta of each particle in the fluid but rather by considering the probability that a number of particles all occupy an arbitrarily small region of space[14]. This is given by the probability function $f = f(t, x, v)$ in the 6-dimensional phase space ($x, v \in R^3$) describing the motion and position of each particle at a given time. From time evolution we can determine how other related physics quantities change as well, such as heat energy, momentum, viscosity or thermal conductivity of a fluid.

The most general form of this equation can be written in Hamiltonian format as:

$$\hat{L}[f] = \hat{Q}[f] \tag{3.1}$$

where \widehat{L} is the Liouville operator describing the evolution of a phase space volume and \widehat{Q} is the collision operator. The (non-relativistic) form of L is:

$$L_{NR} = \frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla + \vec{F} \cdot \frac{\partial}{\partial \vec{p}}$$

Since we have stated that there will be no external force the third term in the Liouville operator disappears[15], arriving to the homogeneous transport equation or also known as Boltzmann equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f) \quad (3.2)$$

The right hand side function $Q(f)$ which is function of $f = f(x, v, t)$ is the collision operator:

$$Q(f)(v) = \iint [f(\vec{v}')f(\vec{v}'_i) - f(\vec{v})f(\vec{v}_i)][(\vec{v} - \vec{v}_i) \cdot \vec{n}] dn_i dv_i \quad (3.3)$$

and has the form:

- Allows only binary collisions $\implies Q(f)$ will be quadratic in f .
- Particles are point-particles $\implies Q(f) = Q(f)(v)$, acts only in v .

And each of its terms in order:

1. Gain term: this first term encapsulates the amount of particles with velocity \vec{v} being created by the collision of particles with velocities \vec{v}' and \vec{v}'_i .
2. Loss term: this second term subtracts from the first term those particles with an initial velocity \vec{v} that have lost it when colliding with particles of velocity \vec{v}_i .
3. Collision cross section: gives the partition of collisions for hard spheres, to differentiate between different times of collision depending on the cross-section in use.
4. Now \vec{n} is an statistical parameter on the sphere of collision since its formal definition here is not necessary since we are treating with point particles.

The Boltzmann equation provides therefore a link from Hamiltonian mechanics to describe with a probabilistic model the behaviour of particles in a fluid at a microscopic level. There is a but to all of this elegance and is the loss of information. The one-particle function distribution has all the information of collisions in the collision term ($Q(f)$ in eq. 3.2). Nevertheless, the collision term therefore is dependent on the two-particle probability function, and the two-particle is also dependent on the three, and so on by induction. Therefore, it is only possible to actually compute the one-particle distribution function if the information about higher terms of two-particle function are neglected. This is what makes the Boltzmann equation a non-reversible

statement. Concretely, it is where we choose the particles to be correlated before or after the collision. In equation 3.3 we have stated in the collision operator that particles will be uncorrelated before the collision and will be correlated after the collision. This is the assumption that lead Boltzmann to equation 3.2. Though, we could have supposed that collisions were correlated before the collision and not after, and that would have lead as to what is known as the *Anti-Boltzmann Equation*[16], which will only be transform by changing the sign of the term $\overline{\partial_t}$.

3.2 Conservation Laws

As it was mentioned before, the Boltzmann equation can be used to derive other physical quantities. Furthermore, it leads to the fluid dynamic conservation laws for mass, charge, momentum and energy.

This is possible since the transport equation provides a time-development method to track the probability of each of the particles. One more characteristic that has to be added to the picture is their completely interchangeable nature. There exist a symmetry due to this indistinguishable characteristic between \vec{v}_i and \vec{v}_j , for all i and j. Therefore we could rewrite ¹:

$$\int Q(f, f)\Phi(v) dv = \frac{1}{2} \int (f(v'')f(v') - f(v)f(v_i))(\Phi(v) + \Phi(v_i))dv dv_i d\Phi$$

If we also consider micro-reversibility where $(v, v', n) \iff (v', v'_i, n)$, then we could rewrite again:

$$\int Q(f, f)\Phi(v) dv = \frac{1}{4} \int (f(v')f(v'_i) - f(v)f(v_i))(\Phi(v) + \Phi(v_i) - \Phi(v') - \Phi(v'_i))dv dv_i d\Phi$$

This integral seems complicated, but if we take $\Phi = 1, v, |v|^2 \implies$ which will be collision invariants, then:

$$\int Q(f, f)\Phi = 0$$

These invariants are reflections of important physical concepts. Going back to the transport equation, if we substitute each of the values of these collision invariants, we obtain the local conservation laws which provide the link to a macroscopic description [?] of the gas:

$\partial_t \int f dv + \nabla_x \int f \cdot v dv = 0$	Conservation of mass
$\partial_t \int f v dv + \nabla_x \int f v \otimes v dv = 0$	Conservation of momentum
$\partial_t \int f v ^2 dv + \nabla_x \int f v v ^2 dv = 0$	Conservation of energy

¹Vector notation will be absent for simplicity but all v are vectors

There are some problems that arise when discussing the closure in kinetic theory and fluid dynamics of this equations. So far, this is a system of linear equations that becomes non-linear when the closure condition over the system is included, therefore the existence of its solutions becomes more complicated. To read more about this see reference [17].

3.3 Equilibrium States

One of the most important features that were studied in the late 20th century when kinetic theory began to play an important role in physics, was its reconciliation with thermodynamics. In principle, classical mechanics and thermodynamics lead to some paradoxes, such as Gibbs [18]. Nevertheless, most of those paradoxes were later dismantled when the concept of entropy and equilibrium were better defined. Crucially, to see that entropy was a property of the macro-state and not of the micro-states of a system, and so the second law of thermodynamics still hold true.

But one of the main questions that is still unresolved nowadays is the tendency to equilibrium. The Equilibrium principle states that[19]: "An isolated system in an arbitrary initial state within a finite fixed volume will spontaneously attain a unique state of equilibrium". These statement can be summarised into three claims:

1. The existence of equilibrium states for isolated systems.
2. Uniqueness of the equilibrium state.
3. Spontaneous approach to equilibrium from non-equilibrium.

Boltzmann already stated that the equilibrium state in thermodynamics was itself a time-asymmetric notion.

Therefore, the description of non-equilibrium states was the main goal in kinetic theory. When parting from the transport equation, if we consider the spatially homogeneous version, the second term in the LHS is zero. The equation is then:

$$\partial_t f = Q(f)$$

We try to minimise the entropy with the local conservation laws from before. Using then the Lagrangian such that:

$$\log f = \alpha + \beta v + \gamma |v|^2 \tag{3.4}$$

Solving this, f takes the form of a Gaussian, as predicted by Maxwell [15], such that:

$$f(v) = \frac{\rho}{2\pi\tau} \exp\left[-\frac{|v \cdot u|^2}{2\tau}\right]$$

This means that near states of equilibrium, all probability functions will tend to be a Gaussian when the conservation laws apply.

3.4 Boltzmann's H theorem

As we have discussed, thermodynamics and statistical mechanics are all to do with the equilibrium properties of systems. Also, Boltzmann already pointed out that settling down to equilibrium clearly involves an arrow of time that distinguishes the future from the past. Yet the underlying classical mechanics is invariant[20]. This is known as Loschmidt's paradox which consist on the following: how to reconcile the time-reversible microscopic dynamics (Liouville's theorem) and the irreversible macroscopic one (Boltzmann equation)[21].

Boltzmann tried attempted to mechanise the second law in his paper "On the mechanical meaning of the 2nd law of the theory of heat" [22]. For this he used H's theorem.

If we integrate and see that if Φ is of the logarithmic form, the integral is always positive:

$$\int Q(f, f) \log(f) dv = \frac{1}{4} \int (f(v)f(v'_i) - f(v)f(v_i)) \left(\log \frac{f(v')f(v'_i)}{f(v)f(v_i)} \right) \cdot n dv dv_i \geq 0 \quad (3.5)$$

Which means that when subtitled in the transport equation:

$$\partial_t \int f \log f dv + \nabla_x \int f \log f v dv \leq 0 \quad (3.6)$$

The $\log f$ term is called the Lyapunov functional and is related to entropy.

In this search of a proof for the second law of thermodynamics, Boltzmann introduced a quantity that he denoted as H such that:

$$H(t) = \int d^3x d^3p f_1(\vec{x}, \vec{p}; t) \log(f_1(\vec{x}, \vec{p}; t)) \quad (3.7)$$

If it is recalled, the definition of thermodynamical entropy of Boltzmann:

$$S = -k_B H \quad (3.8)$$

The H-theorem, first proven by Boltzmann in 1872, is the statement that H always decreases with time. The entropy always increases. Boltzmann looked at the time dependence of this quantity:

$$\frac{dH}{dt} = \int d^3r d^3p (\log f_1 + 1) \frac{\partial f_1}{\partial t} \quad (3.9)$$

We can eliminate the +1 because $\int f_1 = N$ is unchanging, ensuring that $\int \frac{\partial f_1}{\partial t} = 0$. Using the Boltzmann equation (3.2), we have:

$$\frac{dH}{dt} = \int d^3x d^3p \frac{\partial f_1}{\partial t} \cdot \log(f_1) \quad (3.10)$$

For which replacing the value of the partial differential of f_1 seen in Liouville's, we are left to see that the change in H is entirely due to the collision integral factor.

Therefore the change in H is governed by the collision term, which taking the assumption of molecular chaos with pre-collision configurations (such that the velocities before the collision are uncorrelated), he arrived to:

$$\frac{dH}{dt} \leq 0 \implies \frac{dS}{dt} \geq 0 \quad (3.11)$$

Assuming then that collisions are uncorrelated and that f_2 after collision is such that, $f_2 \sim f_1 f_1$. This means that for any macroscopic process, the H quantity will decrease with time as it reaches equilibrium, which means that entropy will increase with time and hence, it could be seen as a justification of the second law of thermodynamics.

4

Incompressible Navier-Stokes

The Navier-Stokes equations can be derived from the basic conservation and continuity equations applied to properties of fluids. In order to derive the equations of fluid motion, we must first derive the continuity equation (which dictates conditions under which things are conserved), apply the equation to conservation of mass and momentum, and finally combine the conservation equations with a physical understanding of what a fluid is.

The continuity equation describes the change of an intensity property L . The volume Ω is assumed to be of any form; its bounding surface area is referred to as $\partial\Omega$ [23]. To derive the continuity equation the first basic assumption is that of Reynold's Transport Theorem, usually symbolised as follows:

$$\frac{d}{dt} \int_{\Omega} L dV = - \int_{\partial\Omega} L \vec{v} \cdot \vec{n} dA - \int_{\Omega} Q dV \quad (4.1)$$

The left hand side of the equation denotes the rate of change of the property L contained inside the volume Ω . The right hand side is the sum of two negative terms:

- A flux term, $\int_{\partial\Omega} L \vec{v} \cdot \vec{n} dA$, which indicates how much of the property L is leaving the volume by flowing over the boundary $\partial\Omega$. Where \vec{v} the average velocity of the macroscopic fluid.
- A sink term, $\int_{\Omega} Q dV$, which describes how much of the property L is leaving the volume due to sinks or sources inside the boundary.

Equation (4.1) states that the change in the total amount of a property is due to how much flows out through the volume boundary as well as how much is lost or gained through sources or sinks inside the boundary. To proceed, we also need the divergence theorem, which allow the flux term of the above equation to be expressed

as a volume integral. Also by Leibniz's Rule, we can put the time derivative inside the integral. Therefore we can write the resulting equation:

$$\int_{\Omega} \frac{dL}{dt} dV = - \int_{\Omega} \nabla \cdot (L\vec{v}) + Q dV \quad (4.2)$$

Which can be rewritten as:

$$\int_{\Omega} \left(\frac{d}{dt} L + \nabla \cdot (L\vec{v}) + Q \right) = 0 \quad (4.3)$$

This relation applies to any control volume Ω ; the only way the above equality remains true for all control volumes is if the integrand itself is zero. Thus, we arrive at the general form of the continuity equation:

$$\frac{dL}{dt} + \nabla \cdot (L\vec{v}) + Q = 0 \quad (4.4)$$

Applying the continuity equation to density (the intensive property equivalent to mass), we obtain

$$\frac{d\rho}{dt} + \nabla \cdot (\rho\vec{v}) + Q = 0. \quad (4.5)$$

This is the same as conservation of mass because we are operating with a constant control volume Ω . With no sources or sinks of mass hence ($Q = 0$),

$$\frac{d\rho}{dt} + \nabla \cdot (\rho\vec{v}) = 0.$$

This is the equation of conservation of mass. In some cases, such as when we have a pipe pumping fluid in or out of the system inside the control volume, we might not want to assume that $Q = 0$; however, for the general case, we make the assumption that mass is not added or removed from the system. However, in certain cases it is useful to simplify it further. For an incompressible fluid, the density is constant. Setting the derivative of density equal to zero and dividing through by a constant ρ , we obtain the simplest form of the equation:

$$\nabla \cdot \vec{v} = 0$$

With the concept of conservation of mass and conservation of momentum, we will make a few more assumptions about the forces and the behaviour of fluids, lead to the equations of motion for fluid. We assume that the body force on the fluid parcels is due to two components, fluid stresses and external forces:

$$\vec{b} = \nabla \cdot \sigma + \vec{f}. \quad (4.6)$$

Here, σ is the stress tensor, and \vec{f} represents external forces. Intuitively, the fluid stress is represented as the divergence of the stress tensor because the divergence is the extent to which the tensor acts as a sink or a source; in other words, the divergence

of the tensor results in a momentum source or sink, which is exactly a force. The stress tensor is:

$$\sigma = \begin{bmatrix} \omega_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix}$$

This tensor is divided into two terms of interest in the general form of the Navier-Stokes equation. The two terms are the volumetric stress tensor, which tends to change the volume of the body, and the stress deviator tensor, which tends to deform the body. The volumetric stress tensor represents the force which sets the volume of the body (namely, the pressure forces). The stress deviator tensor represents the forces which determine body deformation and movement, and is composed of the shear stresses on the fluid. Thus, is broken down into:

$$\sigma = \begin{bmatrix} \omega_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} = - \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix} + \begin{bmatrix} \omega_{xx} + p & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} + p & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} + p \end{bmatrix} \quad (4.7)$$

Denoting the stress deviator tensor as T , we can make the substitution:

$$\sigma = -pI + T \quad (4.8)$$

Substituting this into the previous equation, we arrive at the Navier-Stokes Equation:

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \nabla \cdot T + \vec{f}.$$

The physical meaning of each of its terms:

- Left hand side is the force on each fluid particle, composed of three of the RHS terms.
- $-\nabla p$: A pressure term (also known as the volumetric stress tensor) which prevents motion due to normal stresses. The fluid presses against itself and keeps it from shrinking in volume.
- $\nabla \cdot T$: A stress term (known as the stress deviator tensor) which causes motion due to horizontal friction and shear stresses. The shear stress causes turbulence and viscous flows.
- \vec{f} : The force term which is acting on every single fluid particle.

Nevertheless, the most general form of, the Incompressible Navier-Stokes equation in convective form is :

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} - \nu \nabla^2 \vec{u} = -\nabla \omega + \vec{g} \quad (4.9)$$

Where each of the terms:

- $\vec{v} \rightarrow$ flow velocity.
- $\nu \rightarrow$ kinematic viscosity.
- LHS: 1. Variation of velocity. 2. Convection 3. diffusion
- RHS: 1. Internal sinking source 2. External source

Although this is the general form of the Navier-Stokes equation, it cannot be applied until it has been more specified. First off, depending on the type of fluid, an expression must be determined for the stress tensor T ; secondly, if the fluid is not assumed to be incompressible, an equation of state and an equation dictating conservation of energy are necessary. There are usually specific to the fluid which the equation is being applied to. A number of fluid models exist, varying the tensor T and the equation of state (for compressible fluids).

- Newtonian Fluids: Compressible or Incompressible.
- Non-Newtonian Fluids: like Bingham plastics or Power-law Fluids.

The Navier-Stokes equation (4.9) is an irreversible equations. Meaning that it loses information due to the diffusion term. This is the last step in the stairway of the micro-meso-macroscopic.

5

The Bridge: from microscopic to mesoscopic

5.1 BBGKY Hierarchy

As it was seen in section 5, we have build a system with the Liouville equation where we have a description of the system in terms of N-particle phase space distribution. Although we haven't really simplified the situation since we still had N-coupled equations. This was something that we didn't have in Boltzmann equation. The bridge between Classical Mechanics and Kinetic Theory, is what the BBGKY hierarchy is attempting to present. The Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy is a set of equations describing the dynamics of a system of a large number of interacting particles, forming a coupled chain of equations.

Writing the *one-particle distribution*:

$$f_1(\vec{x}, \vec{p}; t) = N \int \prod_{i=2}^N d^3x_i d^3p_i f(\vec{x}, \vec{x}_2, \dots, \vec{x}_N, \vec{p}, \vec{p}_2, \dots, \vec{p}_N; t)$$

With this, we are assuming as before with the billiard balls that all particles are identical. The factor N in the expression is there to ensure normalisation:

$$\int d^3x d^3p f_1(\vec{x}, \vec{p}; t) = N$$

This functions encapsulates all we need to know about the system. Such as density, number of particles or energy. But how does f_1 change with time? The time evolution will be given by the Liouville's equation, such that:

$$\frac{\partial f_1}{\partial t} = N \int \prod_{i=2}^N d^3x_i d^3p_i \frac{\partial f}{\partial t} = N \int \prod_{i=2}^N d^3x_i d^3p_i \{H, f\}$$

Integrating by parts and moving away from f , we can arrive to the expression:

$$\frac{\partial f_1}{\partial t} = \{H_1, f_1\} + N \int \prod_{i=2}^N d^3x d^3p_i \sum_{k=2}^N \frac{\partial U(\vec{x} - \vec{x}_k)}{\vec{x}} \cdot \frac{\partial f}{\partial \vec{p}_i} \quad (5.1)$$

Where we have defined the one-particle Hamiltonian H_1 :

$$H_1 = \frac{p^2}{2m} + V(\vec{r}) \quad (5.2)$$

We should notice that H_1 includes an external force Vacting on the particle, but it does not say anything about the interaction with other particles. All that information is included in the term $U(\vec{r} - \vec{r}_k)$. Therefore we can see that the time-evolution of the one-particle distribution function is a Liouville's like equation with an extra term:

$$\frac{\partial f}{\partial t} = \{H_1, f_1\} + \left(\frac{\partial f_1}{\partial t}\right)_{coll} \quad (5.3)$$

The first term is sometimes referred to as streaming term, and it tells you how the particles move in the absence of collisions. The second term is the collision integral, and is given by the second term in equation (5.3). Also the collision integral cannot be expressed in terms of only the one-particle distribution function. Because f_1 contains no information about where any of the other particles are in relation to the first. However some of that information is contained in the two-particle distribution function, and so on. This way, we need to generalise the expression into the N BBGKY hierarchy equations:

$$f_n(\vec{x}_1, \dots, \vec{x}_n, \vec{p}_1, \dots, \vec{p}_n; t) = \frac{N!}{(N-n)} \int \prod_{i=n+1}^N d^3x_i d^3p_i f(\vec{x}_1, \dots, \vec{x}_n, \vec{p}_1, \dots, \vec{p}_N; t) \quad (5.4)$$

Which obeys the equation:

$$\frac{\partial f_n}{\partial t} = \{H_n, f_n\} + \sum_{n=1}^n \int d^3x_{n+1} d^3p_{n+1} \frac{\partial U(\vec{x}_i - \vec{x}_{n+1})}{\vec{x}_i} \cdot \frac{\partial f_{n+1}}{\partial \vec{p}_i} \quad (5.5)$$

Although at a first glance it doesn't seem as if the problem had been simplified, it is not easier to apply approximations since we have a hierarchy of coupled equations, rather than an equation for each particle.

Low Density Limit

Boltzmann equation is not deterministic. Statistical description starting from system of particles follows trajectories of the Liouville's equations but in a very big space.

$$f_N = (t, x_1, x_2, \dots, x_N, v_1, v_2, \dots, v_N) \partial_t f_N + \sum_{i=1}^N v_i \nabla_{x_i} f_N = 0$$

on domain $D_N = \{|x_i - x_j| > \epsilon\}$ i.e. no overlap + reflection on the boundary of the domain. F_N is symmetric with respect to all $z_i = (x_i, v_i)$ where z_i are points of phase space.

Boltzmann-Grad Scaling \longrightarrow Transport and collision to be comparable. The conditions are only valid for perfect gases:

- $N \longrightarrow \infty$ then $\epsilon \rightarrow 0$
- $N\epsilon^{d-1} \longrightarrow \alpha$
- $N\epsilon^d \longrightarrow 0$

The Boltzmann- Grad Scaling allows therefore a transition between the Hamiltonian description of the system into the kinetic theory. This builds a bridge between the microscopic and mesoscopic description of the system. Once passed through the BBGKY hierarchy, there is similar hierarchy called the Boltzmann hierarchy which leads to the Boltzmann equation, find more on reference: [24]

6

Conclusion

The question of where does irreversibility comes from has been partially answer when we talked about "molecular chaos" assumption made by Boltzmann. We saw that if we were to take the pre-collision configuration instead of the post-collision configuration, we would arrive to a *Anti-Boltzmann* equation that would trace back the trajectories of the particles. Therefore, irreversibility seems to come from this molecular chaos assumption, rather than by mysterious action of an increasing entropy.

Relating to entropy, while the H's theorem seems to resemble the monotonic increasing nature of which entropy is characterised, it does not explain *why* would it be the referred quantity, as it does not explain in the first place why do systems always tend to this equilibrium states the previous discussed Minus First Law), when in thermodynamics this state is a time asymmetric notion by itself. Thus, the H's theorem is not a valid formal proof of the second law of thermodynamics.

It seems that Hilbert presumed the kinetic level of description (the "Boltzmann level") as an intermediate step between the microscopic mechanical description and the continuum mechanics. Nevertheless, this intermediate description may be omitted. But thus only work the recent work of Lanford [25] and his theorem has been able to cross the bridge formally between Hamiltonian mechanics and kinetic theory.

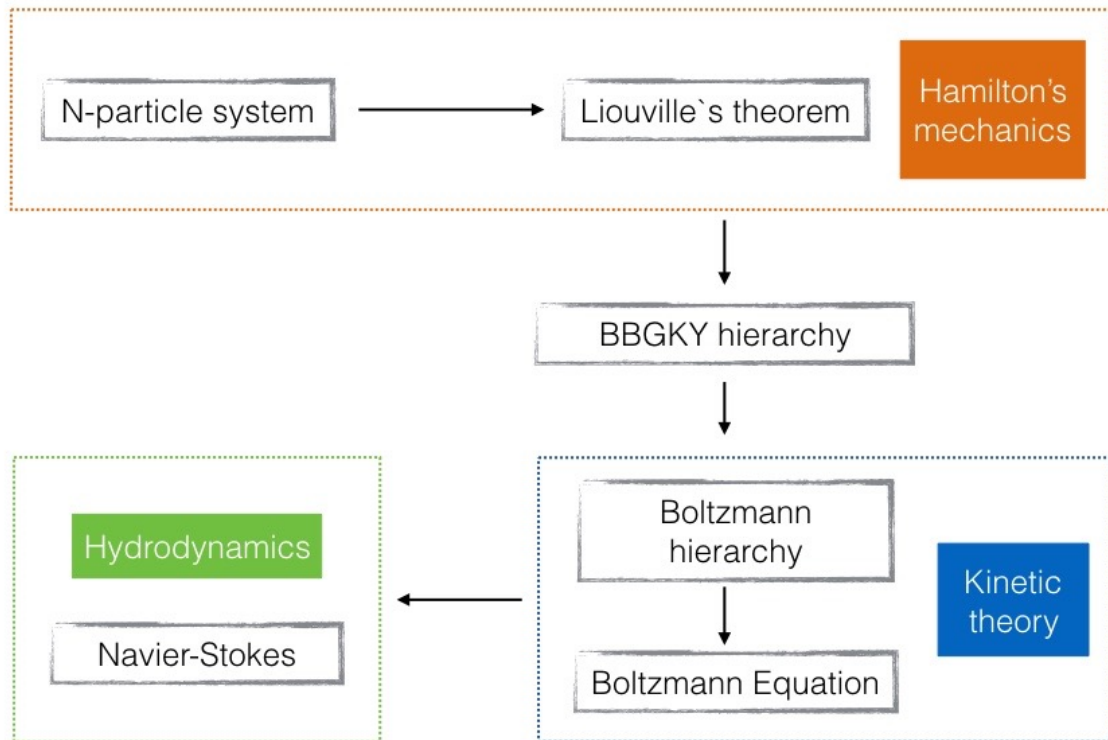
On the other hands, the reduction from the Boltzmann kinetics to hydrodynamics may be split into three problems generally: the existence of hydrodynamics, the form of the hydrodynamic equations and the relaxation of the Boltzmann kinetics to hydrodynamics. Formalisation of these problems is a crucial step in the analysis. Three questions arise: (1) Is there hydrodynamics in the kinetic equation, i.e., is it possible to lift the hydrodynamic fields to the relevant one-particle distribution functions in such a way that the projection of the kinetics of the relevant distributions satisfies some hydrodynamic equations? (2) Do these hydrodynamics have the conventional

Euler and Navier–Stokes– Fourier form? (3) Do the solutions of the kinetic equation degenerate to the hydrodynamic regime (after some transient period)?

The first question is the problem of existence of a hydrodynamic invariant structure for kinetics. The second one is about the form of the hydrodynamic equations obtained by the natural projection of kinetic equations from the invariant structure. The third question is about the step between the relaxation of kinetics to equilibrium, i.e. do solutions to the hydrodynamic equations go fast enough to obtain equilibrium?. All the answers to these questions are only known partially and the bridge between kinetic theory and hydrodynamics are still unresolved.

As a conclusion:

Figure 6.1: Graphical summary of the axiomatization process between scales.



The problem of axiomatising physics will still continue to be unresolved until there is firm bridge between the microscopic and the mesoscopic description, with the Lanford's theorem and BBGKY hierarchy and another pass from mesoscopic and macroscopic one.

References

- [1] Vincent S. Steckline. Zermelo, boltzmann, and the recurrence paradox. 10 December 1982.
- [2] David Hilbert. Mathematical problems. *Bulletin of the American Mathematical Society*, 8(10):437–479, 1902.
- [3] R.P. Feymann. *The character of the physical law*. MIT Press, Cambridge, 1965.
- [4] O. E. Lanford III. *Time evolution of large classical systems*. Springer, Berlin–Heidelberg, 1975.
- [5] I. Gallagher T. Bodineau and L. Saint-Raymond. *The Brownian motion as the limit of a deterministic system of hard-spheres*. Preprint arXiv, 2013.
- [6] David Tong. Classical dynamics. 2005.
- [7] Joel Shapiro. Classical mechanics: Chapter 2, lagrange’s and hamilton’s equations. 1995.
- [8] René Dugas. *A History of Mechanics*. Dover, 1988.
- [9] David Tong. *Lectures in Kinetic Theory*. University of Cambridge, 2012.
- [10] David Cai. Lecture 1: Phase spaces and the liouville equation. Fall 2006.
- [11] Paul Dirac. *Lectures on Quantum Mechanics*. Utrecht University and University of Pittsburgh.
- [12] Peter Woit. *Hamiltonian Mechanics and Symplectic Forms*. Department of Mathematics, Columbia University.
- [13] Benjamin Texier Isabelle Gallagher, Laure Saint-Raymond. *From Newton to Boltzmann: Hard spheres and short-range potentials*.
- [14] P. Mazur S. R. De Groot. *Non-Equilibrium Thermodynamics*. New York: Dover Publications.
- [15] Laure Saint-Raymond. *Mini Course - From particle systems to collisional kinetic equations*.

- [16] P. C. W. Davies. *The Physics of time Asymmetry*. University of California Press, Berkeley and Los Angeles.
- [17] C. David Levermore. *Moment Closure Hierarchies for Kinetic Theories*. Journal of Statistical Physics. Vol. 83, Nos. 5/6, 1996.
- [18] E.T. Jaynes. The gibbs paradox. 7 August 1996.
- [19] Jos Uffink Harvey R. Brown. The origins of time-asymmetry in thermodynamics: The minus first law. 7 August 1996.
- [20] Morinder Singh Modgil. Loschmidt's paradox, entropy and the topology of space-time. 10 August 2009.
- [21] A.S. Trushechkin. Derivation of the boltzmann equation and entropy production in functional mechanics. 2011.
- [22] E.G.D. Cohen. Boltzmann and statistical mechanics. 14 August 1996.
- [23] Marshall Slemrod. *The Problem with Hilbert's 6th Problem*. Mathematical Institute, University of Oxford, 2014.
- [24] Andrea Puglisi. The Boltzmann hierarchy and the Boltzmann equation. <http://denali.phys.uniroma1.it/puglisi/thesis/node23.html>, 2001. [2001-11-14].
- [25] Giovanni Valente Jos Uffink. *Time's arrow and lanford's theorem*. Utrecht University and University of Pittsburgh.
- [26] Harvey R. Brown and Jos Uffinkw. The Origins of Time-Asymmetry in Thermodynamics: The Minus First Law. *Stud. Hist. Phil. Mod. Phys.*, 32(4):525–538, 2001.
- [27] Francois Golse. *De Newton à Boltzmann et Einstein: validation des modèles cinétiques et de diffusion*. Séminaire BOURBAKI.
- [28] Dr Alfred Huan. *Statistical Mechanics*. University of Oxford.
- [29] Clément Mouhot. *Mathematical Topics in Kinetic Theory*. University of Cambridge.
- [30] Harold Grad. *The Many Faces of Entropy*.
- [31] E.T. Jaynes. *The Gibb's Paradox*. Department of Physics. Washington University.
- [32] Fracois Golse. *The Boltzmann Equation and Its Hydrodynamic Limits*. Institut Universitaire de France and Laboratoire Jacques-Louis Lions.

- [33] Irene M. Gamba. *Classical solutions for the Boltzmann transport equations for soft potentials with initial data near local Maxwellians*. Brown University.
- [34] L. Corry. *David Hilbert and the Axiomatization of Physics*, volume 5. 1997.
- [35] A. N. Kolmogorov. *Foundations of the Theory of Probability*. Chelsea, New York, 1950.
- [36] F. Golse C. Bardos and D. Levermore. *Fluid dynamic limits of kinetic equations: Formal derivations*. MIT Press, Cambridge, 1965.
- [37] Thoas Alazard. *A Minicourse on the Low Mach Number Limit*. CNRS University of Paris-Sud 11, France, 1995.
- [38] Sam Punshon-Smith. The boltzmann-grad limit for particles interacting via short-range potentials. 2014.
- [39] Lawrence Sklar. *Physics and Chance*. Cambridge University Press, 1993.